Second Edition

HANDBOOK OF Physical-Chemical Properties and Environmental Fate for Organic Chemicals

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Volume I
Introduction and Hydrocarbons

Volume II
Halogenated Hydrocarbons

Volume III
Oxygen Containing Compounds

Volume IV
Nitrogen and Sulfur Containing Compounds
and Pesticides

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Wan Ying Shiu
Kuo-Ching Ma
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Taylor & Francis
Taylor & Francis Group

Boca Raton London New York

A CRC title, part of the Taylor & Francis imprint, a member of the Taylor & Francis Group, the academic division of T&F Informa plc.

Published in 2006 by
CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

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CRC Press is an imprint of Taylor & Francis Group

No claim to original U.S. Government works
Printed in the United States of America on acid-free paper
10 9 8 7 6 5 4 3 2 1

International Standard Book Number-10: 1-56670-687-4 (Hardcover)
International Standard Book Number-13: 978-1-56670-687-2 (Hardcover)
Library of Congress Card Number 2005051402

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Library of Congress Cataloging-in-Publication Data

Handbook of physical-chemical properties and environmental fate for organic chemicals.--2nd ed. / by Donald Mackay ... [et al.].
p. cm.
Rev. ed. of: Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals / Donald Mackay, Wan Ying Shiu, and Kuo Ching Ma. c1992-c1997.
Includes bibliographical references and index.
ISBN 1-56670-687-4 (set : acid-free paper)
1. Organic compounds--Environmental aspects--Handbooks, manuals, etc. 2. Environmental chemistry--Handbooks, manuals, etc. I. Mackay, Donald, 1936- II. Mackay, Donald, 1936- Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals.

TD196.O73M32 2005
628.5'2--dc22 2005051402

T&F informa
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Preface

This handbook is a compilation of environmentally relevant physical-chemical data for similarly structured groups of chemical substances. These data control the fate of chemicals as they are transported and transformed in the multimedia environment of air, water, soils, sediments, and their resident biota. These fate processes determine the exposure experienced by humans and other organisms and ultimately the risk of adverse effects. The task of assessing chemical fate locally, regionally, and globally is complicated by the large (and increasing) number of chemicals of potential concern; by uncertainties in their physical-chemical properties; and by lack of knowledge of prevailing environmental conditions such as temperature, pH, and deposition rates of solid matter from the atmosphere to water, or from water to bottom sediments. Further, reported values of properties such as solubility are often in conflict. Some are measured accurately, some approximately, and some are estimated by various correlation schemes from molecular structures. In some cases, units or chemical identity are wrongly reported. The user of such data thus has the difficult task of selecting the "best" or "right" values. There is justifiable concern that the resulting deductions of environmental fate may be in substantial error. For example, the potential for evaporation may be greatly underestimated if an erroneously low vapor pressure is selected.

To assist the environmental scientist and engineer in such assessments, this handbook contains compilations of physical-chemical property data for over 1000 chemicals. It has long been recognized that within homologous series, properties vary systematically with molecular size, thus providing guidance about the properties of one substance from those of its homologs. Where practical, plots of these systematic property variations can be used to check the reported data and provide an opportunity for interpolation and even modest extrapolation to estimate unmeasured properties of other substances. Most handbooks treat chemicals only on an individual basis and do not contain this feature of chemical-to-chemical comparison, which can be valuable for identifying errors and estimating properties. This most recent edition includes about 1250 compounds and contains about 30 percent additional physical-chemical property data. There is a more complete coverage of PCBs, PCDDs, PCDFs, and other halogenated hydrocarbons, especially brominated and fluorinated substances that are of more recent environmental concern. Values of the physical-chemical properties are generally reported in the literature at a standard temperature of 20 or 25°C. However, environmental temperatures vary considerably, and thus reliable data are required on the temperature dependence of these properties for fate calculations. A valuable enhancement to this edition is the inclusion of extensive measured temperature-dependent data for the first time. The data focus on water solubility, vapor pressure, and Henry's law constant but include octanol/water and octanol/air partition coefficients where available. They are provided in the form of data tables and correlation equations as well as graphs.

We also demonstrate in Chapter 1 how the data may be taken a stage further and used to estimate likely environmental partitioning tendencies, i.e., how the chemical is likely to become distributed between the various media that comprise our biosphere. The results are presented numerically and pictorially to provide a visual impression of likely environmental behavior. This will be of interest to those assessing environmental fate by confirming the general fate characteristics or behavior profile. It is, of course, only possible here to assess fate in a "typical" or "generic" or "evaluative" environment. No claim is made that a chemical will behave in this manner in all situations, but this assessment should reveal the broad characteristics of behavior. These evaluative fate assessments are generated using simple fugacity models that flow naturally from the compilations of data on physical-chemical properties of relevant chemicals. Illustrations of estimated environmental fate are given in Chapter 1 using Levels I, II, and III mass balance models. These and other models are available for downloading gratis from the website of the Canadian Environmental Modelling Centre at Trent University (www.trent.ca/cemc).

It is hoped that this new edition of the handbook will be of value to environmental scientists and engineers and to students and teachers of environmental science. Its aim is to contribute to better assessments of chemical fate in our multimedia environment by serving as a reference source for environmentally relevant physical-chemical property data of classes of chemicals and by illustrating the likely behavior of these chemicals as they migrate throughout our biosphere.

Acknowledgments

We would never have completed the volumes for the first and second editions of the handbook and the CD-ROMs without the enormous amount of help and support that we received from our colleagues, publishers, editors, friends, and family. We are long overdue in expressing our appreciation.

We would like first to extend deepest thanks to these individuals: Dr. Warren Stiver, Rebecca Lun, Deborah Tam, Dr. Alice Bobra, Dr. Frank Wania, Ying D. Lei, Dr. Hayley Hung, Dr. Antonio Di Guardo, Qiang Kang, Kitty Ma, Edmund Wong, Jenny Ma, and Dr. Tom Harner. During their past and present affiliations with the Department of Chemical Engineering and Applied Chemistry and/or the Institute of Environment Studies at the University of Toronto, they have provided us with many insightful ideas, constructive reviews, relevant property data, computer know-how, and encouragement, which have resulted in substantial improvements to each consecutive volume and edition through the last fifteen years.

Much credit goes to the team of professionals at CRC Press/Taylor & Francis Group who worked on this second edition. Especially important were Dr. Fiona Macdonald, Publisher, Chemistry; Dr. Janice Shackleton, Input Supervisor; Patrica Roberson, Project Coordinator; Elise Oranges and Jay Margolis, Project Editors; and Marcela Peres, Production Assistant.

We are indebted to Brian Lewis, Vivian Collier, Kathy Feinstein, Dr. David Packer, and Randi Cohen for their interest and help in taking our idea of the handbook to fruition.

We also would like to thank Professor Doug Reeve, Chair of the Department of Chemical Engineering and Applied Chemistry at the University of Toronto, as well as the administrative staff for providing the resources and assistance for our efforts.

We are grateful to the University of Toronto and Trent University for providing facilities, to the Natural Sciences and Engineering Research Council of Canada and the consortium of chemical companies that support the Canadian Environmental Modelling Centre for funding of the second edition. It is a pleasure to acknowledge the invaluable contributions of Eva Webster and Ness Mackay.

Biographies

Donald Mackay, born and educated in Scotland, received his degrees in Chemical Engineering from the University of Glasgow. After working in the petrochemical industry he joined the University of Toronto, where he taught for 28 years in the Department of Chemical Engineering and Applied Chemistry and in the Institute for Environmental Studies. In 1995 he moved to Trent University to found the Canadian Environmental Modelling Centre. Professor Mackay's primary research is the study of organic environmental contaminants, their properties, sources, fates, effects, and control, and particularly understanding and modeling their behavior with the aid of the fugacity concept. His work has focused especially on the Great Lakes Basin; on cold northern climates; and on modeling bioaccumulation and chemical fate at local, regional, continental and global scales.

His awards include the SETAC Founders Award, the Honda Prize for Eco-Technology, the Order of Ontario, and the Order of Canada. He has served on the editorial boards of several journals and is a member of SETAC, the American Chemical Society, and the International Association of Great Lakes Research.

Wan-Ying Shiu is a Senior Research Associate in the Department of Chemical Engineering and Applied Chemistry, and the Institute for Environmental Studies, University of Toronto. She received her Ph.D. in Physical Chemistry from the Department of Chemistry, University of Toronto, M.Sc. in Physical Chemistry from St. Francis Xavier University, and B.Sc. in Chemistry from Hong Kong Baptist College. Her research interest is in the area of physical-chemical properties and thermodynamics for organic chemicals of environmental concern.

Kuo-Ching Ma obtained his Ph.D. from Florida State University, M.Sc. from The University of Saskatchewan, and B.Sc. from The National Taiwan University, all in Physical Chemistry. After working many years in the aerospace, battery research, fine chemicals, and metal finishing industries in Canada as a Research Scientist, Technical Supervisor/Director, he is now dedicating his time and interests to environmental research.

Sum Chi Lee received her B.A.Sc. and M.A.Sc. in Chemical Engineering from the University of Toronto. She has conducted environmental research at various government organizations and the University of Toronto. Her research activities have included establishing the physical-chemical properties of organochlorines and understanding the sources, trends, and behavior of persistent organic pollutants in the atmosphere of the Canadian Arctic.

Ms. Lee also possesses experience in technology commercialization. She was involved in the successful commercialization of a proprietary technology that transformed recycled material into environmentally sound products for the building material industry. She went on to pursue her MBA degree, which she earned from York University's Schulich School of Business. She continues her career, combining her engineering and business experiences with her interest in the environmental field.

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5 Halogenated Aliphatic Hydrocarbons

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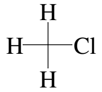
5.1 LIST OF CHEMICALS AND DATA COMPILATIONS

5.1.1 CHLOROALKANES AND CHLOROALKENES

5.1.1.1 Chloromethane (Methyl chloride)



Common Name: Chloromethane
Synonym: methyl chloride, monochloromethane
Chemical Name: chloromethane
CAS Registry No: 74-87-3
Molecular Formula: CH_3Cl
Molecular Weight: 50.488

Melting Point (°C):

–97.7	(Lide 2003)

Boiling Point (°C):

–24.09	(Lide 2003)

Density (g/cm^3 at 20°C):

0.9159	(Dreisbach 1961; Horvath 1982; Weast 1982–83)
0.9214, 0.9111	(20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm^3/mol):

55.0	(calculated-density, Wang et al. 1992)
50.6, 48.8, 54.3, 50.4	(exptl., Tyn and Calus method, Schroeder method, Le Bas method, Reid et al. 1987)
50.5	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

19.06, 21.45	(at 25°C, at normal boiling point, Dreisbach 1961)
18.92, 21.40	(25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.43	(Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

7400	(30°C at 1 atm, McGovern 1943)
5346	(gravitational method, Glew & Moelwyn-Hughes 1953)
6450	(20°C, Dean 1973)
7250	(20°C under 101.3 kPa pressure of CH_3Cl, McConnell et al. 1975; Pearson & McConnell 1975)
6270, 5380	(20, 25°C literature average at 760 mmHg, Dilling 1977)
5325*	(summary of literature data, temp range 5–80°C, Horvath 1982)
4800	(Dean 1985)
6480	(30°C, quoted, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

98048*	(248.9 K, static-manometer, measured range 191.4–248.9 K, Messerly & Aston 1940)
101325*	(–24.0°C, summary of literature data, temp range –99.58 to 24.0°C, Stull 1947)
559860	(interpolated from graph, temp range –50 to 60°C, McGovern 1943)
100800	(Glew & Moelwyn-Hughes 1953)
574500	(calculated-Antoine eq., Dreisbach 1959; 1961)

$\log (P/\text{mmHg}) = 6.99445 - 902.451/(243.63 + t/°C)$; temp range –80 to 3°C (Antoine eq. for liquid state, Dreisbach 1959; 1961)

log (P/mmHg) = 6.99445 – 902.451/(243.60 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
1081* (29.43°C, concentration ratio, measured range 29.43–40.59°C, Swain & Thornton 1962)
539300 (20–25°C, calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 5375.3/(T/K)] + 7.546207; temp range –99 to 137.5°C (Antoine eq., Weast 1972–73)
567900, 576300 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 6.98762 – 899.739/(242.921 + t/°C); temp range –69.2 to –23°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
log (P/mmHg) = 6.09349 – 948.582/(249.336 + t/°C); temp range –75.2 to 5°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
574600 (selected lit., Riddick et al. 1986)
log (P/kPa) = 6.16533 – 920.86/(245.58 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/mmHg) = 7.09349 – 948.58/(249.34 + t/°C); temp range –77 to –5°C (Antoine eq., Dean 1985, 1992)
572800 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.11935 – 902.451/(–29.55 + T/K); temp range 180–266 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.04835 – 869.887/(–33.773 + T/K); temp range 247–310 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.94638 – 1448.913/(47.966 + T/K); temp range 308–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.94022 – 1447.601/(48.385 + T/K); temp range 368–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P/mmHg) = 25.7264 – 1.7503 × 10^3/(T/K) – 6.7151·log (T/K) – 1.2956 × 10^{-9}·(T/K) + 4.4341 × 10^{-6}·$(T/K)^2$; temp range 175–416 K (vapor pressure eq., Yaws 1994)
498820 (293.15 K, selected summary of literature data, temp range 175.44–293.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
953*, 957 (distribution ratio, measured range 4–80°C; calculated-P/C, Glew & Moelwyn-Hughes 1953)
log {H/(mmHg·L/mol)} = 71.005 – 21.656·log (T/K) – 4043.9/(T/K); temp range 277.24–353.23 K (Glew & Moelwyn-Hughes 1953)
1010 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
744, 892 (exptl. as per McConnell et al. 1975, calculated-P/C, Neely 1976)
739 (20°C, Pearson & McConnell 1975)
942 (calculated-C_A/C_W, Dilling 1977)
875 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
log (k_H/atm) = 6.93 – 1248.11/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)
951, 950 (calculated-P/C, recommended, Mackay & Shiu 1981)
894* (EPICS-GC/FID, measured range 10.3–34.6°C, Gossett 1987)
ln [H/(atm m^3/mol)] = 9.358 – 4215/(T/K), temp range: 10.3–34.6°C (EPICS measurements, Gossett 1987)
669 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
867 (computed value, Yaws et al. 1991)
363, 834 (0, 22°C, distilled water, headspace-GC, Elliot & Rowland 1993)
386 (0°C, gas stripping-GC, Moore et al. 1995)
392, 465, 533 (0, 3.0, 6.0°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
ln K_{AW} = 9.17 – 2982/(T/K), seawater of salinity of 30.4‰, temp range: 0–6°C (Moore et al. 1995)
668 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
743 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 3.899 – 1292/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
0.91 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)
0.91 (shake flask, Log P Database, Hansch & Leo 1987)
0.89, 0.936 (calculated-MO, calculated-π substituent const., Bodor et al. 1989)
0.91 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

1.39 (calculated-measured γ^{∞} in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

0.505 (microorganism-water, calculated from K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

0.633 (calculated-K_{OW}, Mabey et al. 1982)
0.778 (selected, Jury et al. 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: half-life of 27–28 min for initial concentration of 1 mg/L in an open container stirred at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);
Evaporation $t_{1/2}$(exptl.) = 27.6 min, $t_{1/2}$(calc) = 0.599 min, 14.9 min from water (Dilling 1977)
$t_{1/2}$ ~ 2.4 h from water (estimated, Thomas 1982);
$t_{1/2}$ ~ 120 d from soil (estimated, Jury et al. 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:
$k_{OH} = 4.7 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}, bimolecular rate constant (Yung et al. 1975)
$k_{OH} = 8.5 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K, bimolecular rate constant with a lifetime $\tau = 0.37$ yr in the troposphere (Cox et al. 1976)
$k_{OH}^* = (4.29 \pm 0.21) \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 250–350 K, with a trospheric lifetime of 1.19 yr (flash photolysis-resonance fluorescence, Davis et al. 1976)
$k_{OH}^* = (4.29 \pm 0.21) \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K with lifetime $\tau = 1.19$ yr, measured range 250–350 K (flash photolysis-resonance fluorescence, Davis et al. 1976; quoted, Altshuller 1980)
$k_{OH} = (3.6 \pm 0.8) \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow-LMR, Howard & Evenson 1976a)
$k_{OH}^* = (4.4 \pm 0.5) \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 298.4 K, measured range 298–423 K and the calculated $t_{1/2}$ ~ 0.2 yr in lower troposphere (flash photolysis-RF, Perry et al. 1976)
$k_{OH} = 24.7 \times 10^9$ cm^3 mol^{-1} s^{-1} at 297 K (flash photolysis-resonance absorption, Paraskevopoulos et al. 1981)
$k_{OH} = 5.0 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}, residence time of 231 d, loss of 0.4% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$k_{OH}^* = 3.95 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 293 K, measured range 247–483 K (discharge-flow resonance fluorescence, Jeong & Kaufman, 1982)
k_{OH}(calc) = 2.4×10^{10} cm^3 mol^{-1} s^{-1} at 300 K (Lyman 1982)
k << 360 M^{-1} h^{-1} for singlet oxygen and 0.05 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982)
$k_{OH}^* = 4.36 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989, 1990)
$k_{OH}^* = 4.9 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K, measured range 295–800 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)
$k_{NO3} = 9.8 \times 10^{-17}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (Atkinson 1991)

Hydrolysis: $k = 6.8 \times 10^{-5}$ h^{-1} with hydrolytic $t_{1/2}$ = 417 d at pH 7 and 25°C (Radding et al. 1977; Mabey & Mill 1978; quoted, Callahan et al. 1979; Mabey et al. 1982);
hydrolysis $k = 2.3710^{-8}$ h^{-1} with $t_{1/2}$ 0.93 yr (Mabey & Mill 1978)
$t_{1/2}$ = 7000 h, based on neutral and base catalyzed hydrolysis rate constants at 25°C extrapolated from data obtained at higher temperatures (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation:
$t_{1/2}$(aq. aerobic) = 168–672 h, based on unacclimated aerobic aqueous screening test data for dichloromethane from experiments utilizing selected domestic waste water inoculum (Tabak et al. 1981; quoted, Howard et al. 1991) and activated sludge inoculum (Klecka 1982; quoted, Howard et al. 1991);
$t_{1/2}$(aq. anaerobic) = 672–2688 h, based on estimated aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (Darnall et al. 1976);
tropospheric lifetime of 1.19 yr due to reaction with OH radical (Davis et al. 1976);
estimated residence time to be about 2 yr for the reaction with OH radical in troposphere (Singh et al. 1979);
lifetime τ = 1.19 yr for reaction with OH radical (Altshuller 1980)
residence time of 231 d, loss of 0.4% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
estimated residence time in troposphere to be 1 yr (Lyman 1982);
$t_{1/2}$ = 1472–14717 h, based on photooxidation half-life in air from measured rate constants for reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);
estimated tropospheric lifetimes of 1.3 yr, and 1.54 yr by rigorous calculation (Nimitz & Skaggs 1992).
lifetime for reaction with OH radicals, τ = 11.7 yr for Polar region, τ = 2.2 yr for Middle region and τ = 0.8 yr for Tropical region in the Northern hemisphere; τ = 0.9 yr for Tropical, τ = 3.6 yr for Middle and τ = 12.3 yr for Polar region in the Southern hemisphere; τ = 1.4 yr in the Global atmosphere, based on data from 1981–1996 (Khalil & Rasmussen 1999a)

Surface water: $t_{1/2}$ = 168–672 h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2}$ = 336–1344 h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} > 50$ d (Ryan et al. 1988); estimated $t_{1/2}$ = 120 d for volatilization from soil (Jury et al. 1990); $t_{1/2}$ = 168–672 h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} > 50$ d, subject to plant uptake from soil via volatilization (Ryan et al. 1988).

TABLE 5.1.1.1.1
Reported aqueous solubilities and Henry's law constants of chloromethane (methyl chloride) at various temperatures

$$S/(\text{wt\%}) = 1.4019 - 6.3562 \times 10^{-2}\cdot(t/°C) + 1.71977 \times 10^{-3}\cdot(t/°C)^2 - 2.8262 \times 10^{-5}\cdot(t/°C)^3 + 2.5268 \times 10^{-7}\cdot(t/°C)^4 - 9.3470 \times 10^{-10}\cdot(t/°C)^5 \quad (1)$$

Aqueous solubility		**Henry's law constant**					
Horvath 1982		**Glew & Moelwyn-Hughes 1953**		**Swain & Thornton 1962**		**Gossett 1987**	
summary of literature data		**concentration ratio**		**concentration ratio**		**EPICS-GC**	
t/°C	**S/g·m^{-3}**	**t/°C**	**H/(Pa m^3/mol)**	**t/°C**	**H/(Pa m^3/mol)**	**t/°C**	**H/(Pa m^3/mol)**
5	14019	4.09	437	29.44	1081	10.3	396.2
10	9113	10.17	568	29.44	1085	17.5	591.7
20	6274	15.06	681	29.44	1073	24.8	893.7
25	5325	20.03	816	29.43	1080	34.6	1256.4
30	4579	25.01	957	29.43	1084		
40	3490	39.91	1475	40.34	1465	ln H = A – B/(T/K)	
50	2742	49.78	1860	40.35	1459		H/(atm m^3/mol)
60	2228	59.99	2260	40.35	1460	A	8.637
70	1891	70.06	2746	40.59	1791	B	4128
80	1609	80.08	3173				
		25.0	956				
eq.1	S/wt%						
		log H = A – B·log (T/K) – C/(T/K)					
			P/(mmHg·L/mol)				
		A	59.096				
		B	21.656				
		C	4043.9				

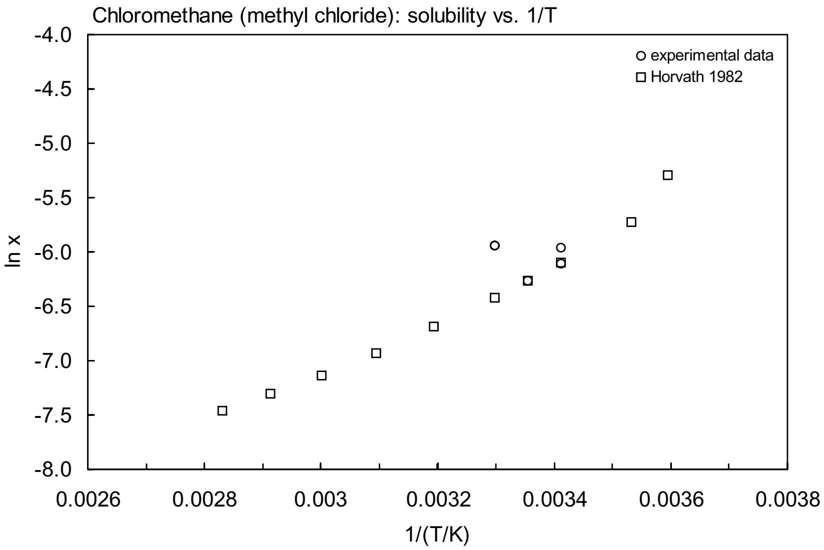


FIGURE 5.1.1.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for chloromethane.

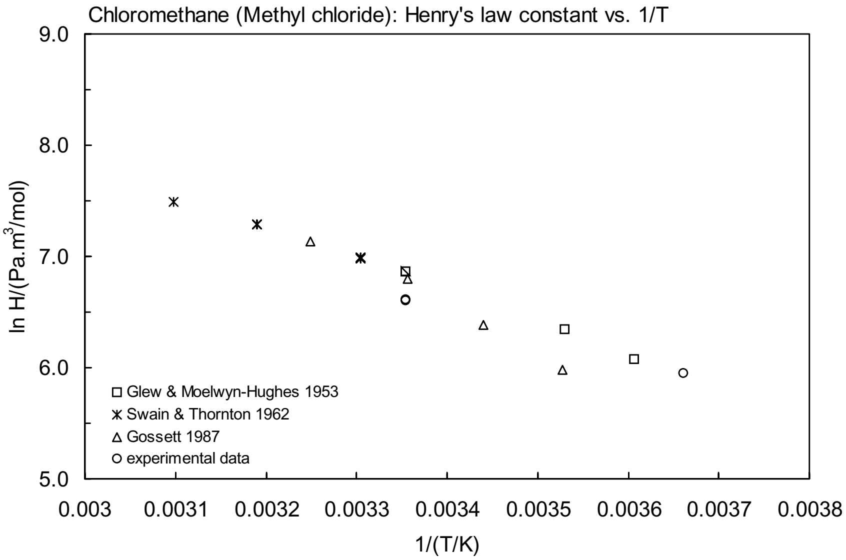


FIGURE 5.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for chloromethane.

TABLE 5.1.1.1.2
Reported vapor pressures of chloromethane (methyl chloride) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log (T/K)$ (4)
$\log P = A - B/(T/K) - C\cdot\log (T/K) + D\cdot(T/K)$ (5)

Messerly & Aston 1940				Stull 1947	
static-manometer				summary of literature data	
T/K	P/Pa	T/K	P/Pa	t/°C	P/Pa
191.424	3509	248.998	101521	-	
191.378	3498	248.943	98048	–99.58	666.6
194.556	4474			–92.4	1333
199.272	6338	eq. 5	P/mmHg	–84.8	2666
206.324	10320	A	31.07167	–76.0	5333
213.539	16343	B	1822.60	–70.4	7999
213.526	16328	C	9.287119	–63.0	13332
222.999	28384	C	0.00555556	–51.2	26664
230.184	41739			–38.0	53329
237.125	59004	mp/K	175.44	–24.0	101325
242.845	77224	bp/K	248.94		
246.441	90805	ΔH_V/(kJ mol^{-1}) = 0.945		mp/°C	–97.7

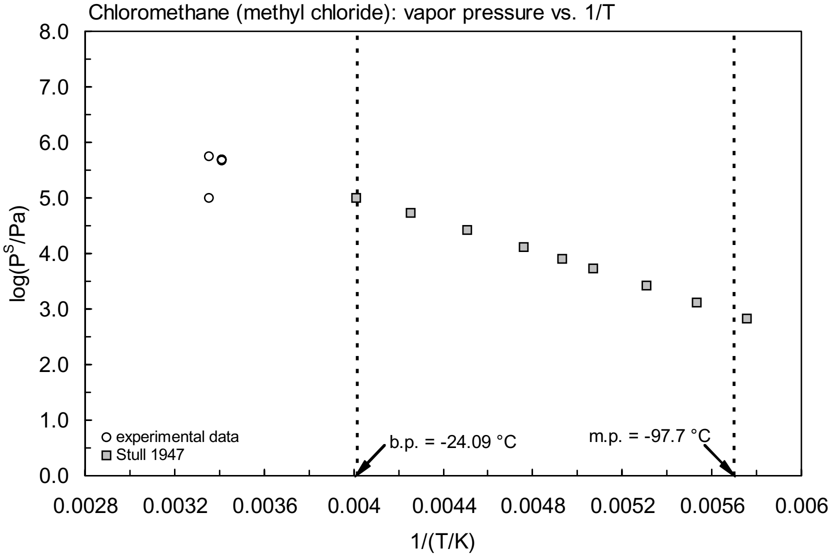
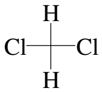


FIGURE 5.1.1.1.3 Logarithm of vapor pressure versus reciprocal temperature for chloromethane.

5.1.1.2 Dichloromethane



$$\mathrm{Cl}-\overset{\mathrm{H}}{\underset{\mathrm{H}}{\mathrm{C}}}-\mathrm{Cl}$$

Common Name: Dichloromethane
Synonym: methylene chloride, methylene dichloride, methane dichloride, methylene bichloride
Chemical Name: dichloromethane
CAS Registry No: 75-09-2
Molecular Formula: CH_2Cl_2
Molecular Weight: 84.933
Melting Point (°C):
–95.2 (Lide 2003)
Boiling Point (°C):
40 (Lide 2003)
Density (g/cm^3 at 20°C):
1.3255, 1.3163 (20°C, 25°C, Dreisbach 1959; 1961)
1.3266 (Horvath 1982; Weast 1982–83)
1.3256, 1.131678 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
64.0 (calculated-density, Wang et al. 1992)
71.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
28.56, 28.98 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
1.435 (calculated, Dreisbach 1959; 1961)
1.472 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are complied at the end of this section):
20000* (20°C, volumetric method, Rex 1906)
19910 (Seidell 1940)
13200 (25°C, data presented between 0–50°C in graph, McGovern 1943)
34480 (shake flask-residue volume method, Booth & Everson 1948)
13200 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
20000* (Archer & Sterns 1977; Andelman 1978; measured range 0–30°C, quoted, Horvath 1982)
22700, 19400 (1.5, 20°C, literature average, Dilling 1977)
13700 (shake flask-titration/turbidity, Coca et al. 1980)
13030* (summary of literature data, Horvath 1982)
13000 (selected, Thomas 1982; Riddick et al. 1986; Howard 1990)
16700 (Verschueren 1983; selected, Valsaraj 1988)
19020 (calculated-UNIFAC activity coeff., Banerjee 1985)
17200* (26.8°C, shake flask-GC/TC, measured range 0–35.7°C, Stephenson 1992)
19260, 19830, 19500, 19500 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
18080, 19995, 20880, 21850 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
20080, 18800, 18880 (10, 20, 30°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
18650 (gas stripping-GC, Li et al. 1993)
20340 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
46510, 68170 (20°C, 30°C, Rex 1906)
57120 (interpolated from graph, temp range –40 to 110°C, McGovern 1943)

57480* (Antoine eq. regression, temp range –70 to 40.7°C, Stull 1947)
58100 (calculated-Antoine eq., Dreisbach 1959; 1961)
log (P/mmHg) = 7.07138 – 1134.6/(231.0 + t/°C); temp range –28 to 121°C (Antoine eq. for liquid state, Dreisbach 1955)
49704* (21.199°C, temp range –9.03 to 39.429°C, Boublik 1960; quoted, Boublik et al. 1984)
70530* (29.993°C, temp range 29.993–39.993°C, Mueller & Ignatoswski 1960)
log (P/mmHg) = 7.0803 – 1138.91/(231.45 + t/°C); temp range –28 to 73°C (Antoine eq. for liquid state, Dreisbach 1961)
57390 (calculated-Antoine eq., temp range –70 to 40.7°C, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 7572.3/(T/K)] + 8.18330; temp range –70 to 40.7°C (Antoine eq., Weast 1972–73)
58275, 57270 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 9.72567 – 2979.516/(395.553 + t/°C); temp range 30–40°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
48200 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
21065, 57062 (1.5, 25°C, Dow Chemicals data, Dilling 1977)
57950, 57980 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.96841 – 1014.441/(216.227 + t/°C); temp range 30–40°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.18791 – 1127.232/(229.764 + t/°C); temp range –9.05 to 38.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
47990 (selected, Daniels et al. 1985)
log (P/mmHg) = 7.4092 – 1325.9/(252.6 + t/°C); temp range –40 to 40°C (Antoine eq., Dean 1985, 1992)
58100 (selected, Riddick et al. 1986)
log (P/kPa) = 6.07622 – 1070.07/(223.24 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
57990 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.18649 – 1126.53/(–43.46 + T/K); temp range 264–312 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.88926 – 1545.323/(3.375 + T/K); temp range 311–383 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.87285 – 861.817/(–94.102 + T/K); temp range 379–455 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.20540 – 449.586/(–193.701 + T/K); temp range 450–510 K (Antoine eq., Stephenson & Malanowski 1987)
47660, 71000, 85640, 102540 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 32.5069 – 2.5166 × 10^3/(T/K) –8.8015·log (T/K) + 1.2934 × 10^{-10}·(T/K) + 3.3194 × 10^{-6}·$(T/K)^2$; temp range 178–510 K (vapor pressure eq., Yaws 1994)
57844 (selected summary of literature data, temp range 178.25–338.15 K, Xiang 2002)
70486 (30°C, vapor-liquid equilibrium study, Pathare et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
231.3 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
301.0 (McConnell et al. 1975; Pearson & McConnell 1975)
322.3 (calculated, Neely 1976)
292, 271.5 (exptl., calculated-C_A/C_W, Dilling 1977)
111.3 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
log (k_H/atm) = 7.92 – 1821.84/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)
295 (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
295* (24.9°C equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C Leighton & Calo 1981)
ln (k_H/atm) = 17.42 – 3645/(T/K); temp range 1.9–24.9°C (equilibrium cell-concn ratio measurements, Leighton & Calo 1981)
205.7 (calculated-P/C, Mabey et al. 1982)
303.9 (calculated-P/C, Thomas 1982)
229.1 (20°C, EPICS-GC, Lincoff & Gossett 1983)
227.9 (20°C, EPICS-GC, Lincoff & Gossett 1984)

199.6 (20°C, batch air stripping-GC, Lincoff & Gossett 1984)
ln [H/(atm m^3/mol)] = 8.200 – 4191/(T/K); temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)
ln [H/(atm m^3/mol)] = 9.035 – 4472/(T/K); temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)
222.0 (EPICS-GC, Gossett 1987)
173.0* (20°C, EPICS-GC/FID, measured range 9.6–34.6°C, Gossett 1987)
ln [H/(atm m^3/mol)] = 9.843 – 5612/(T/K); temp range: 9.6–34.6°C (EPICS measurements, Gossett 1987)
187.7 (20°C, EPICS, Yurteri et al. 1987)
323 (gas stripping-GC, Warner et al. 1987)
300* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 8.483 – 4268/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
451.1 (calculated-QSAR, Nirmalakhandan & Speece 1988)
202.6 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
254.4 (calculated-P/C, Suntio et al. 1988)
251 (computed value, Yaws et al. 1991)
213, 314, 375, 456 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
128, 209, 308 (10, 20, 30°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
266 (γ^∞ from gas stripping-GC, Li et al. 1993)
16.72, 26.04 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
197 (20°C, inert gas stripping-GC, Hovorka & Dohnal 1997)
244.1 (modified EPICS method-GC, Ryu & Park 1999)
260; 221; 211 (EPICS-GC; quoted lit.; calculated-P/C, David et al. 2000)
220 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 4.561 – 1644/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

1.25 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
1.51 (Hansch & Leo 1979)
1.22 (HPLC-k′ correlation, Hafkenscheid & Tomlinson 1983)
1.25 (HPLC-k′ correlation, Tomlinson & Hafkenscheid 1986)
1.25 (recommended, Sangster 1989)
1.35* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
1.25 (recommended, Hansch et al. 1995)
1.25 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

2.27 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

0.699 (calculated as per Lyman et al. 1982, Howard 1990)
0.778 (microorganism-water, calculated from K_{OW}, Mabey et al. 1982)
0.600 (calculated-MCI χ, Koch 1983)
0.362 (selected, Daniels et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

0.944 (calculated-K_{OW}, Mabey et al. 1982)
1.440 (calculated- MCI χ, Koch 1983; quoted, Bahnick & Doucette 1988)
1.000 (selected, Daniels et al. 1985)
1.390 (calculated-MCI χ, Bahnick & Doucette 1988)

Sorption Partition Coefficient, log K_{OM}:

1.44, 1.23 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$(calc) = 2.23 min (Mackay & Wolkoff 1973; quoted, Dilling et al. 1975; Callahan et al. 1979);

$t_{1/2}$(calc) = 20.7 min (Mackay & Leinonen 1975; quoted, Dilling 1977; Callahan et al. 1979);

$t_{1/2}$(exptl) = (21 ± 3) min for 1 ppm in water at 25°C when stirred at 200 rpm in water (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

evaporation $t_{1/2}$(exptl) = (18.3–25.2) min, $t_{1/2}$(calc) = 2.23 and 20.7 min at 25°C and $t_{1/2}$(exptl.) = 34.9 min, $t_{1/2}$ = 24.5 min at 1.5°C (Dilling 1977)

$t_{1/2}$ ~ 3.0 h from water (estimated, Thomas 1982);

$t_{1/2}$ ~ 100 d from soil (estimated, Jury et al. 1990).

Photolysis: estimated photodecomposition $t_{1/2}$ > 250 h from a simulated environmental sunlight exposure (> 290 nm at 27 ± 1°C) study (Dilling et al. 1976; quoted, Callahan et al. 1979);

photodegradation $t_{1/2}$ = 30–120 d (Darnall et al. 1976; quoted, Daniels et al. 1985);

photocatalyzed mineralization by the presence of TiO_2 with a rate of 1.6 ppm/min per gram of catalyst (Ollis 1985).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = 1.24 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K corresponding to a lifetime of 0.30 yr (relative rate method, Cox et al. 1976; quoted, Callahan et al. 1979)

$k_{OH}* = (1.16 \pm 0.05) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K with lifetime of 0.39 yr, measured range 245–375 K (flash photolysis-resonance fluorescence, Davis et al. 1976)

$k_{OH} = 1.55 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH} = (14.5 \pm 2.0) \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 298.5 K and the calculated tropospheric half-life of ~ 0.05 yr in lower troposphere (flash photolysis-RF, Perry et al. 1976)

$k_{OH} = 1.5 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, residence time of 77 d, loss of 1.3% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH}* = 1.53 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 292 K, measured range 251–455 K (discharge flow-resonance fluorescence, Jeong & Karfman 1982)

k << 360 M^{-1} h^{-1} for singlet oxygen and 0.2 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

k ≤ 0.1 M^{-1} s^{-1} for reaction with O_3 in water as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

photooxidation $t_{1/2}$ = 458–4584 h based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k = 4.0 \times 10^7$ M^{-1} s^{-1} with reference to CH_3CCl_3 (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{OH} = 1.42 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}; k(soln) = 9.6×10^{-14} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}* = 1.42 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH}* = 1.76 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 295 K, measured range 298–775 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)

$k = (9 \pm 6) \times 10^7$ M^{-1} h^{-1} for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

Hydrolysis: a minimum hydrolysis $t_{1/2}$ = 18 months was estimated from aqueous reactivity experiments (Dilling et al. 1975; quoted, Callahan et al. 1979; Howard 1990);

rate constant $k = 3.2 \times 10^{-11}$ s^{-1} with a maximum $t_{1/2}$ = 704 yr for hydrolysis at pH 7 and 25°C was reported from the extrapolated experimental data obtained at 100–150°C (Radding et al. 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

$t_{1/2}$ = 260000 d in natural waters at pH 7 (Capel & Larson 1995)

Biodegradation: completely biodegradable under aerobic conditions with sewage seed or activated sludge between 6 h to 7 d (Rittman & McCarty 1980; Davis et al. 1981; Tabak et al. 1981; Klecka 1982; Stover & Kincannon 1983; quoted, Howard 1990)

$t_{1/2}$(aq. aerobic) = 168–672 h based on unacclimated aerobic screening test data (Kawasaki 1980; Tabak et al. 1981; quoted, Howard et al. 1991); $t_{1/2}$(aq. anaerobic) = 672–2688 h based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

$t_{1/2}$(aerobic) = 7 d, $t_{1/2}$(anaerobic) = 28 d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric $t_{1/2}$ = 33 wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)
disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976)
lifetime of 4.4 yr in troposphere for the reaction with OH radical (Altshuller 1980)
estimated disappearance time to be 12 h to 1.0 year in simulated troposphere chamber (Dilling & Goersch 1979; quoted, Lyman 1982)
residence time of 77 d, loss of 1.3% in 1d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)
estimated residence time in troposphere to be 160–250 d (Lyman 1982);
$t_{1/2}$ = 458–4584 h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991)

Surface water: estimated $t_{1/2}$ = 33–38 d in various locations in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)
$t_{1/2}$ = 168–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
biodegradation $t_{1/2}$(aerobic) = 100 d, $t_{1/2}$(anaerobic) = 400 d, hydrolysis $t_{1/2}$ = 3800 d at pH 7 in natural waters (Capel & Larson 1995)
$t_{1/2}$ = 1–1.2 d for the first days up to 4 d and 2.71–2.80 d for a period of up to 14 d for disappearance from water calculated from a pseudo first order equation of mesocosms experiment (Merlin et al. 1992)

Ground water: estimated for the first days up to 4 d and $t_{1/2}$ = 2.71–2.80 d for a period of up to 14 d of 10 yr in the ground water of The Netherlands (Zoeteman et al. 1981)
$t_{1/2}$ = 336–1344 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 10–50 d (Ryan et al. 1988);
volatilization $t_{1/2}$ ~ 100 d from soil (Jury et al. 1990);
biodegradation $t_{1/2}$(aerobic) = 1.3 d (0.16 ppm, conc of dichloromethane), $t_{1/2}$ = 9.4 d (0.5 ppm), $t_{1/2}$ = 191.4 d (5 ppm), all in sandy loam soil; $t_{1/2}$ = 54.8 d in sand (0.5 ppm); $t_{1/2}$ = 12.7 d (0.5 ppm) in sandy clay loam soil; $t_{1/2}$ = 7.2 d (0.5 ppm) in clay with 50 d lag and $t_{1/2}$(anaerobic) = 21.5 d (5 ppm) with 70 d lag (Davis & Madsen 1991);
$t_{1/2}$ = 168–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2}$ = 10–50 d, subject to plant uptake in soil via volatilization (Ryan et al. 1988);
$t_{1/2}$ = 0.4–0.5 d to eliminate from small fish (McCarty et al. 1992).

TABLE 5.1.1.2.1
Reported aqueous solubilities of dichloromethane at various temperatures

$$S/(\mathrm{wt\%}) = 1.961 - 4.4883 \times 10^{-2}\cdot(t/°C) + 8.6617 \times 10^{-4}\cdot(t/°C)^2 + 4.9463 \times 10^{-6}\cdot(t/°C)^3 \qquad (1)$$

1.

Rex 1906		Andelman 1978		Horvath 1982		Stephenson 1992	
volumetric method				summary of literature data		shake flask-GC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
0	23630	0	23100	0	19610	0	20300
10	21220	10	20800	10	15938	9.2	19200
20	20000	20	19600	20	13702	17.3	18000
30	19690	25	20000	25	13030	26.8	17200
		30	19000	30	12605	35.7	17700
				40	12350		
				50	12640		
				eq.1	S/wt%		

TABLE 5.1.1.2.1 (*Continued*)

2.

Tse et al. 1992		Wright et al. 1992	
activity coefficient -GC		activity coefficient	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	19260	10	20080
30	19830	20	18880
35	19500	30	18880
40	19500		

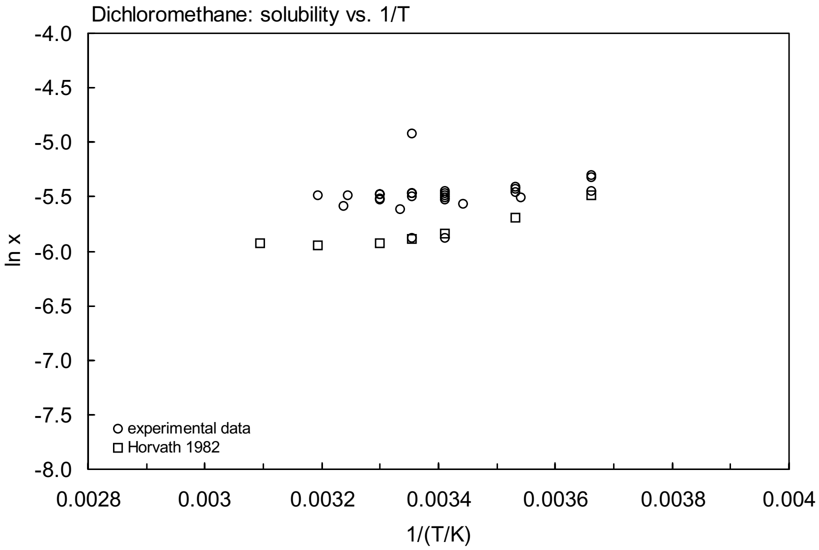


FIGURE 5.1.1.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.2
Reported vapor pressures of dichloromethane at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		

Stull 1947		Mueller & Ignatoswski 1960		Boublik 1960, thesis	
summary of literature data				in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–70.0	133.3	29.993	70530	–9.03	12046
–52.1	666.6	34.993	85175	–5.45	14549
–43.3	1333	38.993	98070	–1.322	17921
–33.4	2666	39.993	102117	2.228	21314
–22.3	5333			6.230	25780
–15.7	7999			9.457	29923
–6.30	13332			13.289	35493

(*Continued*)

TABLE 5.1.1.2.2 (*Continued*)

Stull 1947		Mueller & Ignatoswski 1960		Boublik 1960, thesis	
summary of literature data				in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
8.0	26664			16.693	41470
24.1	53329			21.199	49704
40.7	101325			26.393	61295
				32.337	77123
mp/°C	–96.7			39.429	96484
				eq. 2	P/kPa
				A	6.18791
				B	127.232
				C	229.764
				bp	39.767

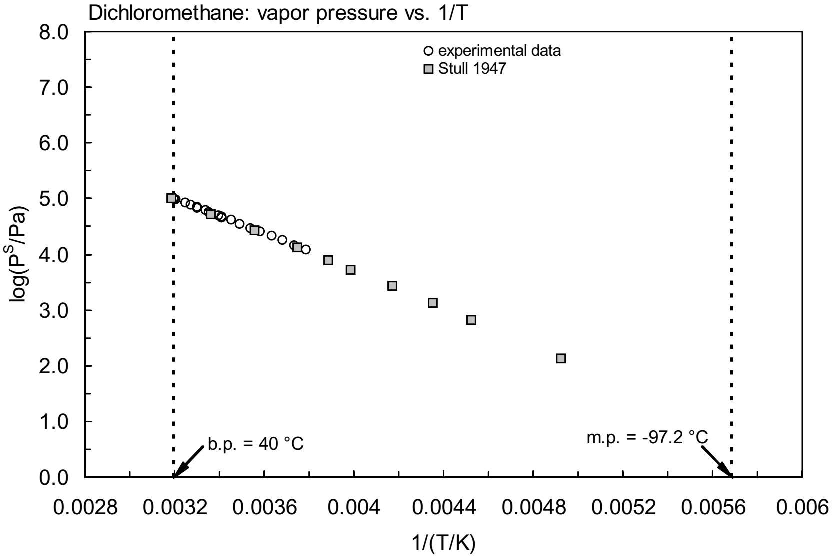


FIGURE 5.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.3
Reported Henry's law constants of dichloromethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tse et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.9	112	9.6	116.5	10	142	20	213
13.5	203	17.5	132.7	15	171	30	314
15.7	222	24.8	221.9	20	247	35	375
22.0	286.5	34.6	330.3	25	300	40	456
24.9	295			30	366		
25	295.3	eq. 4	H/(atm m³/mol)				
		A	6.653	eq. 4	H/(atm m³/mol)	**Wright et al. 1992**	
eq. 3	k_H/atm	B	4215	A	8.483	**activity coefficient**	
A	17.42			B	4268		
B	3645					10	128
						20	209
						30	308

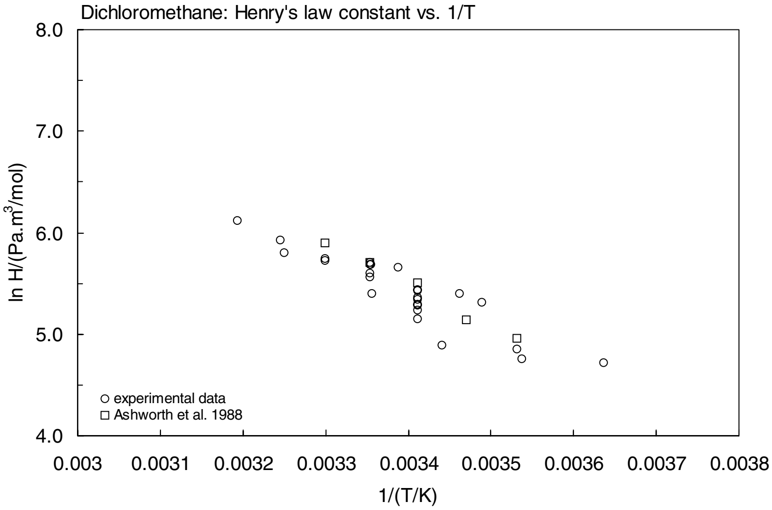


FIGURE 5.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.4
Reported octanol-water partition coefficients of dichloromethane at various temperatures

Bhatia & Sandler 1995	
relative GC-RT technique	
t/°C	log K_{OW}
25	1.35
35	1.34
50	1.37
enthalpy of transfer	
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$	
log $K_{OW} = A - \Delta H/2.303RT$	
A	1.0195
ΔH	–20.2

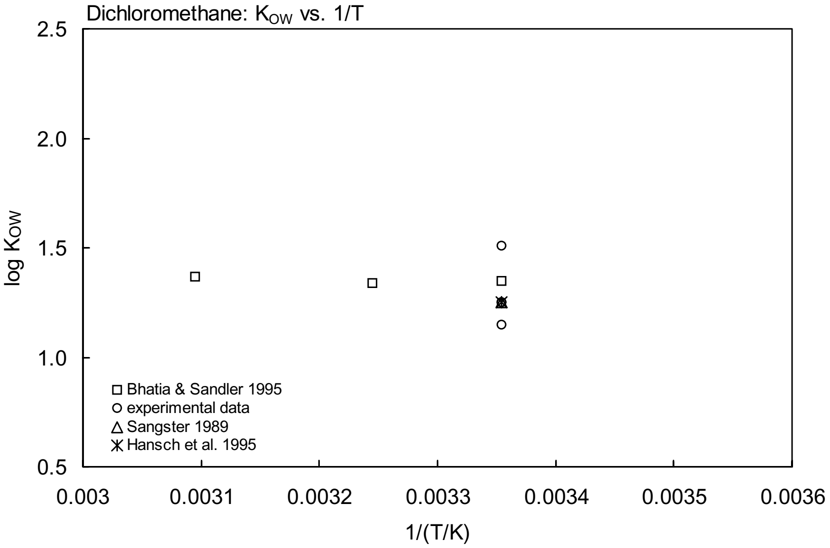
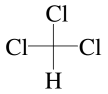


FIGURE 5.1.1.2.4 Logarithm of K_{OW} versus reciprocal temperature for dichloromethane.

5.1.1.3 Trichloromethane (Chloroform)



$$\begin{array}{c} Cl \\ Cl-\overset{|}{\underset{|}{C}}-Cl \\ H \end{array}$$

Common Name: Trichloromethane
Synonym: chloroform, trichloromethaneq
Chemical Name: trichloromethane
CAS Registry No: 67-66-3
Molecular Formula: $CHCl_3$
Molecular Weight: 119.378
Melting Point (°C):
–63.41 (Lide 2003)
Boiling Point (°C):
61.17 (Lide 2003)
Density (g/cm^3 at 20°C):
1.4832 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
1.49845, 1.48911, 1.47970 (15, 20, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
80.0 (calculated-density, Mailhot 1987; Wang et al. 1992)
92.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
33.35, 29.37 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol)
8.80 (calculated, Dreisbach 1959)
9.54 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
8220, 7760 (20°C, 30°C, volumetric method, Rex 1906)
8520, 7710 (15, 30°C, shake flask-interferometer, Gross & Saylor 1931)
8000 (Wright & Schaffer 1932)
7361 (Seidell 1940)
7700 (Seidell 1941)
7900 (data presented from 0–50°C in graph, McGovern 1943)
13320 (shake flask-residue volume method, Booth & Everson 1948)
8000 (20°C, Stephen & Stephen 1963)
8150 (20°C, Riddick & Bunger 1970)
8200 (20°C, Pearson & McConnell 1975)
8000 (20°C, Neely 1976; Verschueren 1977)
10300, 7840 (1.5, 25°C, selected, Dilling 1977)
7230 (shake flask-LSC, Banerjee et al. 1980)
11900 (shake flask-titration/turbidity, Coca et al. 1980)
7360 (shake flask-LSC, Veith et al. 1980)
7920* (summary of literature data, temp range 0–60°C, Horvath 1982)
2525 (30°C, headspace-GC, McNally & Grob 1984)
7190 (calculated-UNIFAC activity coeff., Banerjee 1985)
8200 (shake flask-radiometric method, Lo et al. 1986)
8150 (20°C, selected, Riddick et al. 1986)
8080, 7435, 7290 (20, 35, 50°C, infinite dilution activity coeff. γ^∞-GC, Barr & Newsham 1987)
8670 (23–24°C, shake flask-GC, Broholm et al. 1992)
8200*, 7900 (19.6°C, 29.5°C, shake flask-GC/TC, measured range 0–59.2°C, Stephenson 1992)

7280, 8118, 8558, 9011 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
8108, 7030, 7694 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
7345 (gas stripping-GC, Li et al. 1993)
8098 (20°C, activity coeff. by inert air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
21115, 31990 (20°C, 30°C, Rex 1906)
39345* (35.0°C, vapor-liquid equilibrium, measured range 35.0–60.0°C, Scatchard & Raymond 1938)
26660 (interpolated from graph, temp range –30 to 170°C, McGovern 1943)
25700* (interpolated-Antoine eq. regression, temp range –58.0 to 61.3°C, Stull 1947)
26310 (calculated-Antoine eq., Dreisbach 1959)
$\log (P/mmHg) = 6.90328 - 1163.0/(227.0 + t/°C)$; temp range –15 to 90°C (Antoine eq. for liquid state, Dreisbach 1959)
$\log (P/mmHg) = 6.93708 - 1171.2/(227.0 + t/°C)$; temp range –13 to 97°C (Antoine eq. for liquid state, Dreisbach 1961)
25780* (24.598°C, temp range –10.356 to 60.319°C, Boublik & Aim 1972; quoted, Boublik et al 1984)
23080 (interpolated from Antoine eq., temp range –58 to 254°C, Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 7500.5/(T/K)] + 7.735083$; temp range –58 to 254°C (Antoine eq., Weast 1972–73)
26240, 18950 (calculated-Antoine eq., Boublik et al. 1973)
$\log (P/mmHg) = 6.85465 - 1170.966/(226.252 + t/°C)$; temp range (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log (P/mmHg) = 6.4934 - 959.444/(196.03 + t/°C)$; temp range (Antoine eq. from reported exptl. data, Boublik et al. 1973)
26217, 26104 (static method-differential pressure gauge, Bissell & Williamson 1975)
20000 (20°C, Pearson & McConnell 1975)
25590 (literature average, Dilling 1977)
21330 (20°C, Verschueren 1983)
26220, 32080 (calculated-Antoine eq., Boublik et al. 1984)
21330 (20°C, quoted, McNally & Grob 1984)
$\log (P/mmHg) = 6.4934 - 929.44/(196.03 + t/°C)$; temp range –36 to 61°C (Antoine eq., Dean 1985, 1992)
25970 (selected, Riddick et al. 1986)
$\log (P/kPa) = 5.96288 - 1106.94/(218.552 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
26220 (calculated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.07853 - 1170.42/(-46.98 + T/K)$; temp range 262–334 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 5.38327 - 948.979/(-61.73 + T/K)$; temp range 227–269 K (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.11152 - 1173.606/(-48.54 + T/K)$; temp range 333–416 K (Antoine eq.-III, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 7.89882 - 2879.244/(-161.978 + T/K)$; temp range 410–481 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 4.58922 - 181.802/(-325.74 + T/K)$; temp range 479–523 K (Antoine eq.-V, Stephenson & Malanowski 1987)
$\log (P/mmHg) = 56.6178 - 3.2462 \times 10^3/(T/K) - 18.7 \cdot \log (T/K) + 9.515 \times 10^{-3} \cdot (T/K) + 1.1553 \times 10^{-12} \cdot (T/K)^2$; temp range 210–536 K (vapor pressure eq., Yaws 1994)
26182 (selected summary of literature data, temp range 209.64–368.15 K, Xiang 2002)
32408 (30°C, vapor-liquid equilibrium VLE data, Pathare et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
314.1 (20°C, Dilling et al. 1975)
440.8 (calculated as $1/K_{AW}$, C_W/C_A, Hine & Mookerjee 1975)
283.4 (20°C, McConnell et al. 1975; Pearson & McConell 1975)
310 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

log (k_H/atm) = 9.10 – 2103.09/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)

373* (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)

ln (k_H/atm) = 18.97 – 4046/(T/K); temp range 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

292.0 (20°C, calculated-P/C, Mabey et al. 1982; Mills et al. 1982)

536.9 (batch stripping-GC, Munz & Roberts 1982; Roberts & Dändliker 1983; Roberts et al. 1985)

432.2 (calculated-UNIFAC activity coeff., Arbuckle 1983)

ln K_{AW} = 10.63 – 3649/(T/K); measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith et al. 1983)

298 (calculated-P/C, Jury et al. 1984; Jury et al. 1990)

337.4; 308 (20°C, EPICS-GC; batch air stripping-headspace GC, Lincoff & Gossett 1984)

ln [H/(atm m^3/mol)] = 8.553 – 4180/(T/K); temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)

ln [H/(atm m^3/mol)] = 8.956 – 4322/(T/K), temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)

304; 314; 486, 365 (20°C, batch air stripping-GC; calculated-P/C; quoted lit. values, Nicholson et al. 1984)

334, 294, 314 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)

ln [H/(atm m^3/mol)] = 11.90 – 5200/(T/K); temp range 10–30°C (air stripping-GC, Nicholson et al. 1984)

343.4 (adsorption isotherm, Urano & Murata 1985)

372* (EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)

ln [H/(atm m^3/mol)] = 9.843 – 4612/(T/K); temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)

334 (EPICS-GC, Munz & Roberts 1987)

log K_{AW} = 4.990 – 1729/(T/K), temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

343 (gas stripping-GC, Warner et al. 1987)

427; 387; 372; 374; 399 (EPICS-GC; calculated-P/C; EPICS; direct concn ratio; calculated-UNIFAC activity coefficient, Ashworth et al. 1988)

427* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm·m^3/mol)] = 11.41 – 5030/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

294 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

318 (calculated-P/C, Suntio et al. 1988; Mackay & Shiu 1990)

411 (computed value, Yaws et al. 1991)

199.3* (26.5°C, tap water, EPICS-GC, measured range 26.5–47.2°C, Tancréde & Yanagisawa 1990)

log K_{AW} = 9.154 – 3051/(T/K); temp range 26.5–47.2°C (EPICS measurements, Tancréde & Yanagisawa 1990)

306, 592, 1046 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)

362 (activity coefficient γ^∞ from gas stripping-GC, Li et al. 1993)

514, 513 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

379* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)

177, 444 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)

ln K_{AW} = –4142/(T/K) + 0.00588·Z + 12.012; with Z salinity of 0–35.5‰ and temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)

212, 341 (10, 20°C, gas stripping-GC, Moore et al. 1995)

126, 214, 352 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

ln K_{AW} = 11.17 – 3840/(T/K); seawater of salinity of 30.4‰, temp range: 0–20°C (Moore et al. 1995)

261, 451 (15, 25°C, vapor liquid equilibrium-GC, Turner et al. 1996)

K_{AW} = 0.0394 + 0.00486·(T/K); temp range 0–60°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)

312 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)

331.2 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

370.8 (modified EPICS method-GC, Ryu & Park 1999)

411; 260 (EPICS-GC; calculated-P/C, David et al. 2000)

307 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 5.343 – 1830/(T/K) (summary of literature data, Staudinger & Roberts 2001)

704.5 (37°C, equilibrium headspace-GC, Batterman et al. 2002)

408* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)

ln K_{AW} = 10.96 – 3821.3/(T/K); temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

1.97 (Hansch & Anderson 1967)
1.97 (shake flask-UV, Hansch et al. 1968; Leo et al. 1971; Hansch et al. 1975)
1.94 (Hansch & Leo 1979)
1.90 (shake flask-LSC, Banerjee et al. 1980)
1.90 (shake flask-LSC, Veith et al. 1980)
1.81 (HPLC-k′ correlation, McDuffie 1981)
2.15 (HPLC-k′ correlation, Wells et al. 1981)
1.91 (calculated-UNIFAC activity coeff., Arbuckle 1983)
1.90 (HPLC-k′ correlation, Hafkenscheid & Tomlinson 1983)
2.14, 2.13, 2.03 (HPLC-k′ correlation, Tomlinson & Hafkenscheid 1986)
1.66 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
1.97 (recommended, Sangster 1989)
2.00* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
1.86* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

2.80 (equilibrium head-space-GC, Abraham et al. 2001)
2.55; 2.53 (equilibrium headspace-GC; calculated-K_{OW}/K_{AW}, Batterman et al. 2002)

Bioconcentration Factor, log BCF:

0.92 (calculate-K_{OW}, Veith et al. 1979; quoted, Veith et al. 1980)
0.78 (bluegill sunfish, Barrows et al. 1980; Bysshe 1982)
0.78 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982; quoted, Davies & Dobbs 1984; Suntio et al. 1988; Isnard & Lambert 1988; Saito et al. 1992)
0.63 (calculated-K_{OW}, Mackay 1982)
1.41 (microorganisms-water, calculated from K_{OW}, Mabey et al. 1982)
0.97 (calculated-MCI χ, Koch 1983)
0.78 (bluegill sunfish, LSC, Davies & Dobbs 1984)
2.84 (green algae, Mailhot 1987)
2.84 (*Selenastrum capricornutum*, Mailhot 1987)
0.52–1.01; 0.204–0.40; 0.46–0.49; 0.552–0.57 (rainbow trout; bluegill sunfish; large mouth bass; catfish, Howard 1990)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

1.64 (calculated-K_{OW}, Mabey et al. 1982)
1.65 (calculated-MCI χ, Koch 1983)
2.15 (wastewater solids with correlation to K_{OW} Dobbs et al. 1989)
1.44 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
1.98 (20°C, weathered shale, mudrock, sorption isotherm-headspace method, Grathwohl 1990)
2.79 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
1.85, 1.92 (20°C, calculated-K_{OW}, Grathwohl 1990)
1.53 (soil, Howard 1990)
1.46 (selected, Jury et al. 1990)
1.57; 1.46; 1.54 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
1.63, 1.65, 1.63, 1.66, 1.69, 1.65, 1.70 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon f_{OC} = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)

Sorption Partition Coefficient, log K_{OM}:

1.65, 1.40 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: calculated $t_{½}$ = 1.4 min (Mackay & Wolkoff 1973);

primary transport process from the aquatic environment with $t_{½}$ = 21–26 min at pH 7 and 25°C stirred at 200 rpm in an open container (Dilling et al. 1975)

evaporation rate k(exptl) = 13.2×10^{-5} g cm^{-2} s^{-1} to still air (Chiou & Freed 1977; Chiou et al. 1980)

evaporation $t_{½}$(exptl) = (8.5–25.7) min, $t_{½}$(calc) = 1.46, 2.37 min at 20–25°C, $t_{½}$(exptl) = 34.6 min at 1.5°C (Dilling 1977)

$t_{½}$ = 3–5.6 h for different laboratory studies of evaporation from water with moderate mixing conditions (Smith et al. 1980; Rathbun & Tai 1981; Lyman et al. 1982; quoted, Howard 1990);

$t_{½}$ = 1.2 d in Rhine River and $t_{½}$ = 31 d in a lake in Rhine Basin. (Zoeteman et al. 1980).

$t_{½}$ ~ 3.7 h from water (estimated, Thomas 1982);

$t_{½}$ = 29 min-11.3 d from rivers and streams, calculated using published O_2 reaeration values; and $t_{½}$(calc) = 31.2 h from rivers and streams, calculated using estimated O_2 reaeration rate constant (Kaczmar et al. 1984);

predicted $t_{½}$ = 36 h in a river, $t_{½}$ = 40 h in a pond and $t_{½}$ = 9–10 d in a lake (USEPA 1984; quoted, Howard 1990);

$t_{½}$ = 4 h at 20°C was predicted from a model river of 1 m deep at flowing speed of 1 m/s with a wind velocity of 3 m/s and its Henry's law constant (Smith et al. 1980; quoted, Howard 1990);

Photolysis: not important only by UV in the stratosphere (Robbins 1976);

probably not significant in aquatic systems (Callahan et al. 1979);

photocatalyzed mineralization by the presence of TiO_2 with a rate of 4.4 ppm min^{-1} g^{-1} of catalyst (Ollis 1985).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{OH} = 1.01×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298 K (discharge flow-LMR, Howard & Evenson 1976a)

k_{OH}* = 1.14×10^{-13} cm^3·$molecule^{-1}$ s^{-1} at 298 K with lifetime of 0.56 yr, measured range 245–375 K (flash photolysis-resonance fluorescence, Davis et al. 1976; quoted, Altshuller 1980)

troposphere with $t_{½}$ = 0.19–0.32 yr due to reaction with OH radical (Callahan et al. 1979)

k_{OH} = 1.0×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, residence time of 116 d, loss of 0.9% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

k_{OH}* = 1.01×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 249–487 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1982)

k_{OH} = 6.6×10^{10} cm^3 mol^{-1} s^{-1} of estimated at 300 K (Lyman 1982)

$t_{½}$ = 78.5–3140 yr from the rate constant for the reaction with OH radical (estimated, Dorfman & Adams 1973)

k << 360 M^{-1} h^{-1} for singlet oxygen and 0.7 M^{-1} h^{-1} for peroxy radical both at 25°C (Mabey et al. 1982)

k ≤ 0.1 M^{-1} s^{-1} for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

photooxidation $t_{½}$ = 26–260 d, based on measured data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

k = 4.0×10^{7} M^{-1} s^{-1} with reference to CH_3CCl_3 (Buxton et al. 1988; quoted, Haag & Yao 1992)

k_{OH} = 1.03×10^{-12} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 1.8×10^{-14} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

k_{OH}* = 1.03×10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 295 K, measured range 295–775 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)

k = $(5.4 \pm 3.0) \times 10^{7}$ M^{-1} s^{-1} for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

k_{OH}* = 1.03×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

Hydrolysis: first-order rate constant k = 0.045 mo^{-1} with $t_{½}$ ~15 months (Dilling et al. 1975; quoted, Callahan et al. 1979);

k = 6.9×10^{-12} s^{-1} (Radding 1976);

hydrolysis rate constant k = 6.9×10^{-12} s^{-1} with $t_{½}$ = 3500 yr at 25°C and pH 7 (Mabey & Mill 1978)

no hydrolysis in acidic aqueous solutions, and rate constant in alkaline aqueous solution, k = 0.23 M^{-1} h^{-1} at 25°C, and k = 2.5×10^{-9} M^{-1} h^{-1} at 25°C in neutral aqueous solutions (Mabey & Mill 1978; Mabey et al. 1982; Mills et al. 1982);

probably not a significant fate process with $t_{1/2}$ = 3500 yr, based on reported rate constant k = 6.9×10^{-12} s^{-1} at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Haque et al. 1980).

Biodegradation: very slow by BOD bottle experiments (Pearson & McConnell 1975);

$t_{1/2}$(aq. aerobic) = 4 wk to 6 months by unacclimated screening tests (Kawasaki 1980; Flathman & Dahlgran 1982; quoted, Howard et al. 1991);

$t_{1/2}$(aq. anaerobic) = 1–4 wk by unacclimated anaerobic screening tests (Bouwer et al. 1981; Bouwer & McCarty 1983; quoted, Howard et al. 1991);

k = 0.5 d^{-1} (Tabak et al. 1981; Mills et al. 1982).

Bioaccumulation: weak to moderate bioaccumulation; no evidence of biomagnification of trichloromethane in marine food chain (Callahan et al. 1979).

Bioconcentration, Uptake(k_1) and Elimination(k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2}$ = 23 wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

residence time of 1.7 yr in troposphere, based on one compartment nonsteady state model (Singh et al. 1978; quoted, Lyman 1982);

residence time of 116 d, loss of 0.9% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

estimated residence time in N. troposphere to be 100 d (Lyman 1982);

$t_{1/2}$ = 623–6231 h, based on photooxidation half-life in air from measured reaction data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

tropospheric lifetime ~ 0.17 yr (estimated, Nimitz & Skaggs 1992)

lifetime for reaction with OH radicals, τ = 3.0 yr for Polar region, τ = 0.6 yr for Middle region and τ = 0.2 yr for Tropical region in the Northern hemisphere; τ = 0.3 yr for Tropical, τ = 1.0 yr for Middle and τ = 3.2 yr for Polar region in the Southern hemisphere; τ = 0.5 yr in the Global atmosphere, based on data from 1985–1996 (Khalil & Rasmussen 1999b)

Surface water: not important for aqueous phase (Dilling et al. 1975);

$t_{1/2}$ = 1.0–31 d in various location in the Netherlands in case of a first order reduction process (estimated, Zoeteman et al. 1980)

$t_{1/2}$ = 672–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2}$ = 1344–43200 h, based on unacclimated aqueous aerobic biodegradation and grab sample data of aerobic soil from a ground water aquifer (Wilson et al. 1983; quoted, Howard et al. 1991).

Soil: $t_{1/2}$ = 10–50 d (Ryan et al. 1988);

$t_{1/2}$ = 100 d, estimated volatilization loss from soil (Jury et al. 1990)

disappearance $t_{1/2}$ = 4.1 d was calculated from first order kinetic for volatilization loss from soil mixtures (Anderson et al. 1991);

$t_{1/2}$ = 672–4320 h, based on estimated aqueous aerobic biodegradation (Howard et al. 1991).

Biota: $t_{1/2}$ < 1 d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{1/2}$ = 10–50 d, subject plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.3.1
Reported aqueous solubilities of trichloromethane at various temperatures

$$S/(\text{wt\%}) = 0.995 - 1.0531 \times 10^{-2} \cdot t/°C + 7.9819 \times 10^{-5} \cdot (t/°C)^2 + 6.6431 \times 10^{-7} \cdot (t/°C)^3 \qquad (1)$$

1.

Rex 1906		Gross & Saylor 1931		Horvath 1982		Barr & Newsham 1987	
volumetric method		shake flask-IR		summary of literature data		activity coefficient	
t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$
20	8220	15	8520	0	9905	20	8080
30	7760	30	7710	10	8983	35	7435
				20	8216	50	7290
				25	7920		
				30	7689		
				40	7440		
				50	7511		
				60	7940		
				eq.1	S/wt%		

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
shake flask-GC		activity coefficient		activity coefficient	
t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$
0	10200	20	7280	20	8108
9.5	9300	30	8118	35	7030
19.6	8200	35	8558	50	7694
29.5	7900	40	9011		
39.3	7400				
49.2	7700				
59.2	7900				

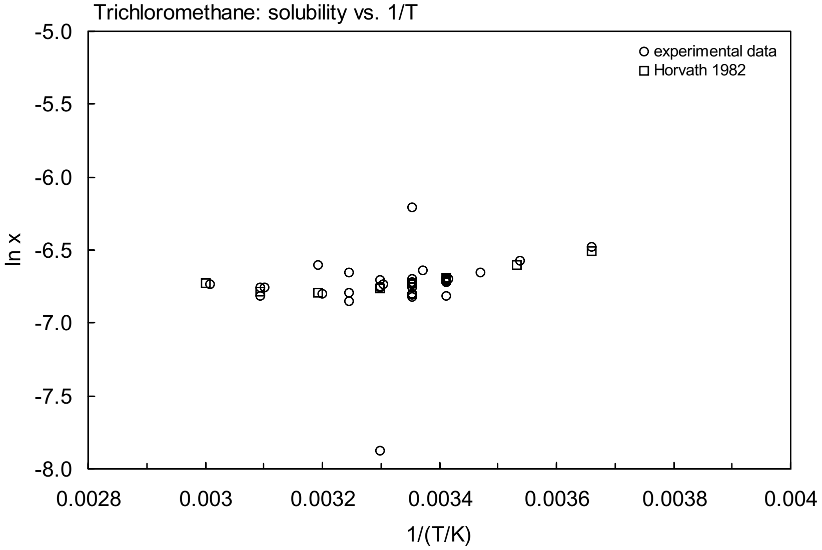


FIGURE 5.1.1.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for trichloromethane.

TABLE 5.1.1.3.2
Reported vapor pressures of trichloromethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Scatchard & Raymond 1938		Stull 1947		Boublik & Aim 1972			
vapor-liquid equilibrium		summary of literature data		in Boublik et al 1984			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
35.0	39345	–58.0	133.3	–10.356	4524	46.583	61295
40.0	48023	–39.1	666.6	–2.610	6967	53.070	77125
45.0	57800	–29.7	1333	2.882	9306	60.319	98412
50.0	69218	–19.0	2666	8.010	12046		
55.0	82372	–7.10	5333	11.927	14549	bp/°C	61.203
60.0	97342	0.50	7999	16.417	17921	Antoine eq	P/kPa
		10.4	13332	20.240	21314	eq. 2	6.07945
		25.9	26664	24.598	25780	A	1170.902
		42.7	53329	28.118	29923	B	226.224
		61.3	101325	32.289	35493	C	
				36.223	41470		
		mp/°C	–65.3	40.913	49704		

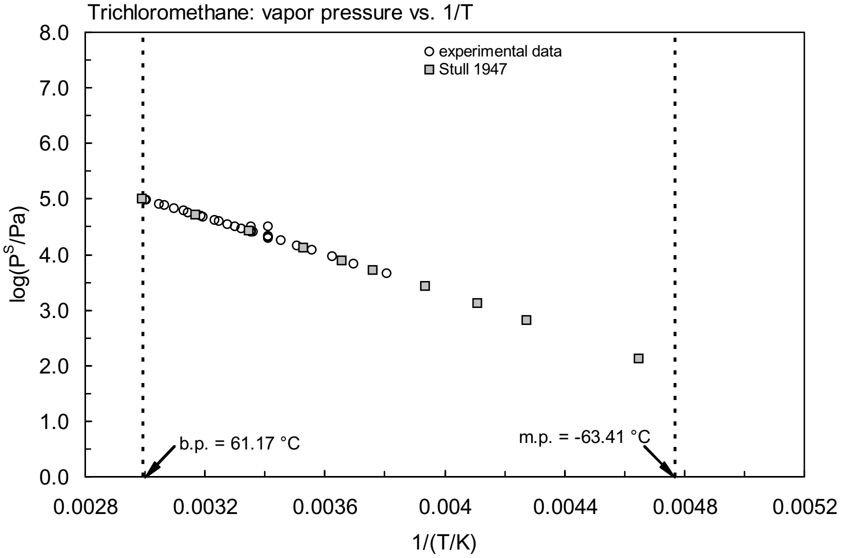


FIGURE 5.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for trichloromethane.

TABLE 5.1.1.3.3
Reported Henry's law constants of trichloromethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)
$\ln H = A - B/(T/K)$ (4) $\log H = A - B/(T/K)$ (4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

1.

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancréde & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.90	125.7	9.6	152	10	174	26.5	199.3
13.5	234.7	17.5	249.3	15	236	27.4	274.9
15.7	267.6	24.8	371.9	20	336	28.9	401.8
17.1	282.7	34.6	570.5	25	427	28.9	276.2
22.0	354.7			30	561	29.7	226.6
24.9	373.5	eq. 4	H/(atm m³/mol)			29.9	277.2
25	373	A	9.843	eq. 4	H/(atm m³/mol)	33.3	382.2
		B	4612	A	11.41	35.6	693.1
eq. 3	k_H/atm			B	5030	38.3	517.9
A	18.97					40	624.8
B	4046					44.7	951.2
						45	925.8
						47.2	1145
						eq. 1	K_{AW}
						A	9.154
						B	3051

2.

Wright et al. 1992		Dewulf et al. 1995		Moore 1995		Görgényi et al. 2002	
activity coefficient		EPICS-GC		gas stripping-GC		EPICS-SPME method	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
20	306	2	116	10	212	2	108
35	592	6	135.1	20	341	6	151.3
50	1046	10	165.7			10	181.3
		18.2	276.1	In sea water 30.4‰ NaCl		16	297.8
		25	379.3	0	126	25	407.5
Bhatia & Sandler 1995				10	214	35	526.5
activity coefficient		eq. 1	K_{AW}	20	352	40	769.9
35	514	A	12.012			50	1120
50	513	B	4142			60	1497
				Turner et al. 1996			
				vapor liquid equilibrium-GC		eq. 1	K_{AW}
				15	261	A	10.96
				25	451	B	3821.3

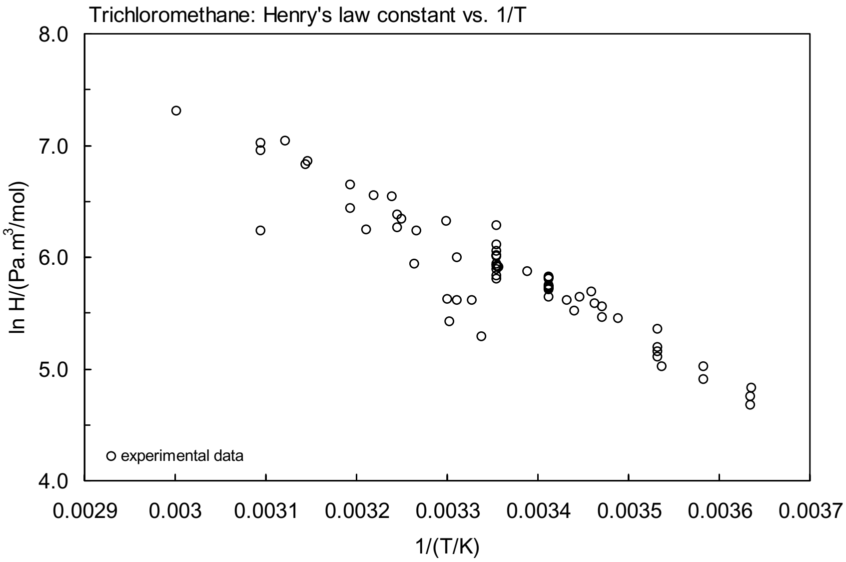


FIGURE 5.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for trichloromethane.

TABLE 5.1.1.3.4
Reported octanol-water partition coefficients of trichloromethane at various temperatures

Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		EPICS-GC	
t/°C	log K_{OW}	t/°C	log K_{OW}
25	2.00	2.2	1.83
35	2.01	6.0	1.815
50	2.00	10.0	1.90
		14.1	1.87
enthalpy of transfer		18.7	1.92
$\Delta H/(kJ\ mol^{-1}) = -20.2$		24.8	1.86
log $K_{OW} = A - \Delta H/2.303RT$		change in enthalpy:	
A	1.0195	$\Delta H_{OW}/(kJ\ mol^{-1}) = 4.2$	
ΔH	–20.2	(–4.4 to 12.8)	
		enthalpy of transfer	
		$\Delta H_{oct}/(kJ\ mol^{-1}) = 0.7$ (–7.9 to 9.3)	

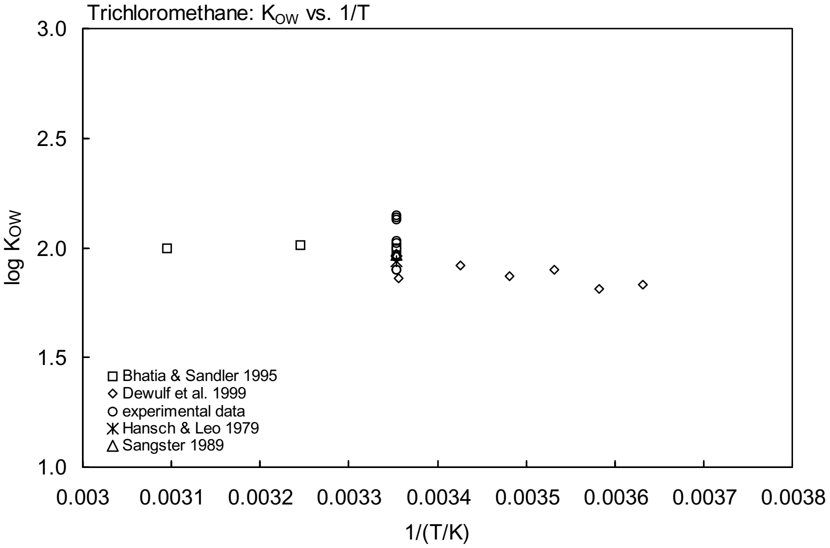
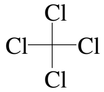


FIGURE 5.1.1.3.4 Logarithm of K_{OW} versus reciprocal temperature for trichloromethane.

5.1.1.4 Tetrachloromethane (Carbon tetrachloride)



Common Name: Carbon tetrachloride
Synonym: tetrachloromethane, methane tetrachloride, perchloromethane, benzinoform
Chemical Name: tetrachloromethane
CAS Registry No: 56-23-5
Molecular Formula: CCl_4
Molecular Weight: 153.823
Melting Point (°C):
–22.62 (Lide 2003)
Boiling Point (°C):
76.8 (Lide 2003)
Density (g/cm^3 at 20°C):
1.594 (McGovern 1943; Dreisbach 1959, 1961; Weast 1982–83; Horvath 1982; Riddick et al. 1986)
1.6037, 1.59402, 1.58436 (15, 20, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
113.2 (calculated-Le Bas method at normal boiling point)
96.0 (calculated-density, Wang et al. 1992)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
32.41, 29.96 (25°C, bp, Riddick et al.1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
0.775 (calculated, Dreisbach 1959)
0.581 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
800, 850 (20°C, 30°C, volumetric method, Rex 1906)
770 (shake flask-interferometer, Gross 1929a,b)
770, 810 (15, 30°C, shake flask-interferometer, Gross & Saylor 1931)
780 (Seidell 1941)
800 (data presented in graph, temp range 0–70°C, McGovern 1943; Dilling 1977)
770 (15°C, Jones et al. 1957)
785 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
778 (20°C, recommended, Sørensen & Arit 1979)
800* (measured range 20–30°C, Andelman 1978)
757 (shake flask-LSC, Banerjee et al. 1980)
700 (shake flask-titration/turbidity, Coca et al. 1980)
793.4* (summary of literature data, Horvath 1982)
831 (calculated-UNIFAC activity coeff., Arbuckle 1983)
753 (calculated-UNIFAC activity coeff., Banerjee 1985)
800 (shake flask-radiometric method, Lo et al. 1986)
770 (selected, Riddick et al. 1986)
780 (23–24°C, shake flask-GC, Broholm et al. 1992)
600*, 720 (20.5, 31.0°C, shake flask-GC/TC, measured range 0–75°C, Stephenson 1992)
930, 873, 950, 982 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
756, 896, 972, 1052 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
700, 652, 652 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
701, 702 (20°C, calculated-activity coefficients, Wright et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

17170, 18810 (20°C, 30°C, Rex 1906)

11372* (19.8°C, manometry, measured range 19.8–76.4°C, Smyth & Engel 1929)

15200 (extrapolated-Antoine eq., vapor-liquid equilibrium VLE data, measured range 30–70°C, Scatchard et al. 1939; quoted, Bissell & Williamson 1975)

log (P/mmHg) = 6.68148 – 1045.022/(T/K) – 99.577/(T/K)^2; temp range 30–70°C (VLE data, Scatchard et al. 1939)

14530 (interpolated from graph, temp range –20 to 170°C, McGovern 1943)

14340* (interpolated from Antoine eq. regression, temp range –50 to 76.7°C, Stull 1947)

15200 (McGlashan et al. 1954)

15100 (Moelwyn-Hughes & Missen 1957)

15360 (calculated-Antoine eq., Dreisbach 1959)

log (P/mmHg) = 6.93390 – 1242.43/(230.0 + t/°C); temp range –15 to 138°C (Antoine eq. for liquid state, Dreisbach 1959)

15372* (25.2°C, temp range 14.06–76.84°C, Boublik 1960; quoted, Boublik et al. 1984)

log (P/mmHg) = 6.94369 – 1221.1/(224.0 + t/°C); temp range –1 to 113°C (Antoine eq. for liquid state, Dreisbach 1961)

15220* (twin ebulliometer, measured range 20–77°C, Hildenbrand & McDonald 1959)

15230 (Marsh 1968; quoted, Bissell & Williamson 1975)

13200 (calculated-Antoine eq., Weast 1972–73)

log (P/mmHg) = [–0.2185 × 7628.8/(T/K)] + 7.586045; temp range –50 to 276°C (Antoine eq., Weast 1972–73)

15250, 15240 (calculated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 6.9218 – 1235.172/(228.957 + t/°C); temp range 19.9–77.7°C (Antoine eq. from reported exptl. data of Hildenbrand & McDonald 1959, Boublik et al. 1973)

log (P/mmHg) = 6.87926 – 1212.021/(226.409 + t/°C); temp range 14.06–76.04°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

15195, 15184 (static method-differential pressure gauge, Bissell & Williamson 1975)

12000 (20°C, Pearson & McConnell 1975

15230 (calculated-Antoine eq., Boublik et al. 1984)

15370, 15300 (25.2°C, quoted exptl., calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.04073 – 1231.791/(228.51 + t/°C); temp range 19.9–77.7°C (Antoine eq. from reported exptl. data of Hildenbrand & McDonald 1959, Boublik et al. 1984)

log (P/kPa) = 5.94824 – 1177.609/(222.028 + t/°C); temp range 40–65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.00535 – 1212.676/(226.483 + t/°C); temp range 14.06–76.04°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

15170 (Daubert & Danner 1985)

log (P/mmHg) = 6.87926 – 1212.021/(226.41 + t/°C), temp range not specified (Antoine eq., Dean 1985, 1992)

15360 (selected, Riddick et al. 1986)

log (P/kPa) = 6.10455 – 1265.632/(232.148 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

15210 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P_S/kPa) = 8.214 – 2027/(T/K); temp range 208–225 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_S/kPa) = 7.946 – 1975.3/(T/K), temp range 226–248 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.99114 – 1202.9/(–48.01 + T/K); temp range 262–249 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.97092 – 1195.9034/(–48.217 + T/K); temp range 349–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.22882 – 1392.458/(–19.19 + T/K); temp range 412–497 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P/mmHg) = 31.9407 – 2.6614 × 10^3/(T/K) –8.5763·log (T/K) – 6.7136 × 10^{-10}·(T/K) + 2.9732 × 10^{-6}·(T/K)^2; temp range 250–556 K (vapor pressure eq., Yaws 1994)

15320 (selected summary of literature data, temp range 250.33–398.15 K, Xiang 2002)

18826 (30°C, vapor-liquid equilibrium study, Pathare et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2912 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

152.8 (calculated-bond method, Hine & Mookerjee 1975)

2216 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)

2776 (gas stripping-GC, Mackay et al. 1979)

2350 (20°C, calculated-P/C, Kavanaugh & Trussell 1980, 1983)

$\log (H/atm) = 10.06 - 2038.25/(T/K)$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)

2797* (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)

$\ln (k_H/atm) = 22.22 - 4438/(T/K)$; temp range 1.0–27.2°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

2160 (calculated-P/C, Mackay & Shiu 1981)

2330 (20°C, calculated-P/C, Mabey et al. 1982)

2454 (20°C, batch stripping, Munz & Roberts 1982)

2418 (20°C, calculated-UNIFAC activity coeff., Arbuckle 1983)

3081 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)

$\ln K_{AW} = 9.77 - 2918/(T/K)$; measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)

$\ln K_{AW} = 11.27 - 3230/(T/K)$; measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith 1983)

3060 (adsorption isotherm, Urano & Murata 1985)

2369 (20°C, multiple equilibration, Munz & Roberts 1986)

3080* (EPICS-GC/FID, Gossett 1987)

2367* (20°C, EPICS-GC/FID, measured range 10.0–34.6°C, Gossett 1987)

$\ln [H/(atm\ m^3/mol)] = 11.29 - 4411/(T/K)$; temp range 10.0–34.6°C (EPICS measurements, Gossett 1987)

2266 (20°C, calculated-P/C, McKone 1987)

3027 (EPICS-GC, Munz & Roberts 1987)

$\log K_{AW} = 5.853 - 1718/(T/K)$; temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

2900 (calculated-P/C, Warner et al. 1987)

228 (20°C, EPICS-GC, Yurteri et al. 1987)

2989* (EPICS-GC, measured range 10–30°C, Ashworth et al. 1988)

$\ln [H/(atm \cdot m^3/mol)] = 9.739 - 3951/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

2330 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

2980 (computed value, Yaws et al. 1991)

2990 (EPICS-GC, Tancréde et al. 1992)

2875* (tap water, EPICS-GC, measured range 25–47.2°C,Tancréde & Yanagisawa 1990)

$\log K_{AW} = 5.569 - 1639/(T/K)$; temp range: 25–47.2°C (EPICS measurements, Tancréde & Yanagisawa 1990)

2067, 3415, 3871, 4580 (20, 30, 35, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)

2646, 4392, 6624 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)

3133* (27.6°C, EPICS-GC, measured range 27.6–45°C, Hansen et al. 1993)

$\ln [H/(kPa \cdot m^3/mol)] = -3553/(T/K) + 13.0$; temp range 27–45°C (EPICS measurements, Hansen et al. 1993)

4.04, 6.0 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

2598* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)

1341, 3370 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)

$\ln K_{AW} = -4073/(T/K) + 0.00814 \cdot Z + 13.772$; with Z salinity 0–35.5‰, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)

2352 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

2612 (modified EPICS method-GC, Ryu & Park 1999)

2313 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{AW} = 5.736 - 1689/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.64 (Leo et al. 1971)

2.62 (shake flask-GC, Chiou et al. 1977)

2.83 (shake flask, Hansch & Leo 1979, 1987)

2.73 (shake flask-LSC, Banerjee et al. 1980)
2.73 (shake flask-LSC, Veith et al. 1980)
2.94 (HPLC-k′ correlation, McDuffie 1981)
2.81, 290 (calculated from UNIFAC activity coeff. with octanol and water mutual solubility considered, not considered, Arbuckle 1983)
2.83 (HPLC-k′ correlation, Hafkenscheid & Tomlinson 1983)
2.03 (HPLC correlation, Eadsforth 1986)
2.73 (HPLC-k′ correlation, Tomlinson & Hafkenscheid 1986)
2.38 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
2.83 (recommended, Sangster 1989)
2.83 (recommended, Hansch et al. 1995)
2.73* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
2.38* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
2.79 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
1.24 (rainbow trout, Neely et al. 1974; Veith et al. 1979)
1.25 (trout muscle, calculated-ratio of rate const. k_1/k_2, Neely et al. 1974)
1.48 (bluegill sunfish, Barrows et al. 1980; Veith et al. 1980; Veith & Kosian 1982)
2.32 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
1.72 (rainbow trout, Veith & Kosian 1982)
2.68 (activated sludge, Freitag et al. 1984)
2.48 (*alga chlorella fusca*-LSC, Geyer et al. 1984)
2.68, 2.48, < 1.0 (activated sludge, *Chlorella fusca*, golden ide, Freitag et al. 1985)
2.06 (calculated-K_{OW}, $S_{OCTANOL}$, and mp, Banerjee & Baughman 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
2.04 (calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.64 (calculated-K_{OW}, Mabey et al. 1982)
1.85 (calculated-MCI χ, Koch 1983)
1.70 (calculated-MCI χ, Bahnick & Doucette 1988)
1.26, 1.34, 1.70, 1.96, 2.07 (DTMA-clay, TTMA-clay, HTMA-clay, BDHA-clay, DDPA-clay, Smith et al. 1990)
1.69 (80% DTMA-clay at 20°C, Smith & Jaffé 1991)
2.16; 1.70; 2.06 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43, weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
2.20, 2.24, 2.24, 2.25, 2.28, 2.27, 2.33 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon f_{OC} = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)‰
1.80, 1.80, 1.78 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
2.01, 2.00, 2.02 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:
1.55 (calculated-MCI χ, Sabljic 1984)
1.89, 1.72 (Florida peat, OC 57.1%; Michigan muck, OC 53.1%, batch equilibrium-sorption equilibrium, Rutherford & Chiou 1992; Rutherford et al. 1992)
0.243, 1.866 (cellulose, extracted peat, Rutherford et al. 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2}$ = 29 min was determined in an open container with initial concentration of 1 mg/L when stirred at 100 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982; Verschueren 1983);
Evaporation $t_{1/2}$(exptl) = 28.8 min, $t_{1/2}$(calc) = 0.2 min, 25.5 min from water (Dilling 1977);

ratio of evaporation rate constant to that of oxygen reaeration: 0.47 as measured value compared to 0.43 as predicted (Smith et al. 1980);

$k < 2.4 \times 10^8$ cm^3 mol^{-1} s^{-1}, estimated rate constant for the reaction with OH radical at 300 K (Lyman 1982);

$t_{1/2}$ ~3.7 h from a model river of 1 m deep for water flowing at 1 m/s with wind speed of 3 m/s and Henry's law constant (Thomas 1982; Lyman et al. 1982; quoted, Howard 1990).

Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 0.18 ppm/min per gram of catalyst (Ollis 1985).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} < 1.2\ 5 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (relative rate method, Cox et al. 1976)

$k_{OH} = 1 \times 10^{-16}$ cm^3 s^{-1} bimolecular reaction rate, with a reported tropospheric lifetime of greater than 330 yr (Cox et al. 1976; quoted, Callahan et al. 1979)

$k_{OH} < 0.1 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH} < 1.0 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1}, residence time > 11600 d, loss ≈ 0.0% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

k_{OH}(calc) << 360 M^{-1} h^{-1} for singlet oxygen and k << 1 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

$k \leq$ 0.005 M^{-1} s^{-1} for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

photooxidation half-life in air: $1.6 \times 10^4 - 1.6 \times 10^5$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k < 2 \times 10^6$ M^{-1} s^{-1} for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

$k_{OH} < 5 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

Hydrolysis: hydrolysis rate constant $k = 4.8 \times 10^{-7}$ s^{-1} with $t_{1/2}$ = 7000 yr (1 ppm), $t_{1/2}$ = 7 yr (1000 ppm) at 25°C and pH 7 (Mabey & Mill 1978)

calculated first-order $t_{1/2}$ = 7000 yr, based on reported rate constant $k = 4.8 \times 10^{-7}$ mol^{-1} s^{-1} for 1 mg/L concentration at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Howard 1990; Howard et al. 1991)

$t_{1/2}$ = 2,600,000 d at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: $t_{1/2}$(aq. aerobic) = 4320–8640 h, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2}$(aq. anaerobic) = 168–672 h, based on unacclimated anaerobic screening test data (Bouwer & McCarty 1983; quoted, Howard et al. 1991) and acclimated anaerobic sediment/aquifer grab sample data (Parsons et al. 1985; quoted, Howard et al. 1991).

$t_{1/2}$(aerobic) = 170 d, $t_{1/2}$(anaerobic) = 7 d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of 1×10^{-10} mL cell^{-1} h^{-1} for bacteria in water (Mabey et al. 1982).

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 4.05 h^{-1}; k_2 = 0.229 h^{-1} (trout muscle, Neely et al. 1974; quoted, Thomann 1989)

k_1 = 4.05 mL g^{-1} h^{-1} (10°C, trout gill, Neely 1979)

k_1 = 4.10 h^{-1}; k_2 = 0.25 h^{-1} (trout, Hawker & Connell 1985)

Half-Lives in the Environment:

Air: tropospheric $t_{1/2}$ = 10 wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2}$ > 10 d for the reaction with OH radical in air (Darnall et al. 1976);

estimated residence time in troposphere, > 330 yr (CEQ 1975);

estimated residence time of 100 yr in troposphere (Singh et al. 1979);

residence time > 11600 d, loss ≈0.0% in 1d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

estimated residence time of 4–20 yr in troposphere (Lyman 1982);

$t_{1/2}$ = 30–50 yr residence time in the troposphere (Howard 1990);

$t_{1/2} = 1.6 \times 10^4 - 1.6 \times 10^5$ h, based on photooxidation half-life in air from measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: estimated $t_{1/2}$ = 0.4–56 d in various locations in the Netherlands in case of a first order reduction process; $t_{1/2}$ ~ 3–30 d in rivers and $t_{1/2}$ = 3–300 d in lakes (Zoeteman et al. 1980);

$t_{1/2}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation (Howard et al. 1991).

$t_{1/2}$(aerobic) = 170 d, $t_{1/2}$(anaerobic) = 7 d in natural waters (Capel & Larson 1995)

Ground water: estimated $t_{1/2}$ ~ 3–300 d (Zoeteman et al. 1980; quoted, Howard 1990);
$t_{1/2}$ = 168–8640 h, based on estimated aqueous aerobic biodegradation half-life and acclimated anaerobic sediment/aquifer grab sample data (Howard et al. 1991).
Sediment:
Soil: $t_{1/2}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
$t_{1/2}$(calc) = 50 d in soil mixtures from first-order kinetic (Anderson et al. 1991).
Biota: $t_{1/2}$ < 1 d in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 5.1.1.4.1
Reported aqueous solubilities of tetrachloromethane at various temperatures

$$S/(\text{wt\%}) = 9.7842 \times 10^{-2} - 1.4942 \times 10^{-3}\cdot(t/°C) + 3.5854 \times 10^{-5}\cdot(t/°C)^2 + 2.2775 \times 10^{-7}\cdot(t/°C)^3 \quad (1)$$

1.

Rex 1906		Gross & Saylor 1931		Andelman 1978		Horvath 1982	
volumetric method		shake flask-IR				summary of literature data	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
20	800	15	770	20	793	0	978.4
30	850	30	810	25	800	10	682.6
				30	814	20	804.8
						25	793.4
						30	791.3
						40	808.6
						50	843.0
						60	880.7
						70	908.1
						eq. 1	S/wt%

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
shake flask-GC		activity coefficient		activity coefficient	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
0	890	20	930	20	700
10	630	30	873	30	652
20.5	600	35	950	40	652
31.0	720	40	982		
41.3	680				
52.5	780				
64.0	960				
75.0	1150				

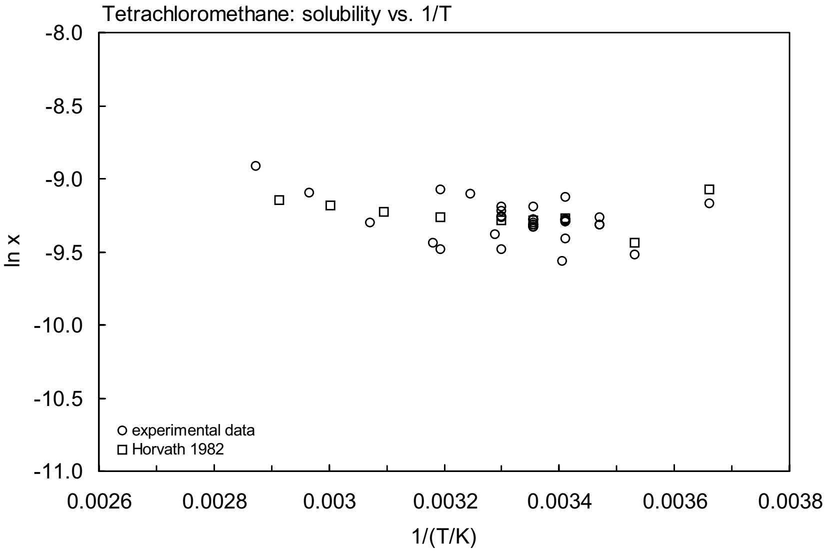


FIGURE 5.1.1.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.2
Reported vapor pressures of tetrachloromethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log(T/K)$ (4)

Smyth & Engel 1929		Stull 1947		Hildenbrand & McDonald 1959		Boublik 1960, thesis	
static-manometer		summary of literature data		twin ebulliometer system		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
19.2	11732	–50.0	133.3	19.88	12079	14.06	9120
32.4	20798	–30.0	666.6	30.93	25211	16.66	10426
41.2	29704	–19.6	1333	56.16	51605	18.46	11876
50.0	41597	–8.20	2666	75.28	96965	21.71	13159
60.8	60368	4.30	5333	76.16	99645	25.2	15372
68.7	78180	12.3	7999	76.87	101729	29.13	18252
76.4	101325	23.0	13332	77.71	104369	33.45	21891
		38.3	26664	76.73	101325	36.98	25264
bp/°C	76.4	57.8	53329			42.07	30864
		76.7	101325	ΔH_V/(kJ mol^{-1}) = 32.41		47.21	37543
					at 25°C	52.36	45367
		mp/°C	–22.6			58.61	56448
				eq. 2	P/mmHg	64.78	69487
				A	6.89406	71.43	86053
				B	1219.58	76.84	99256
				C	227.16		
						bp/°C	76.714
						eq. 2	P/kPa
						A	6.00535
						B	1212.676
						C	226.483

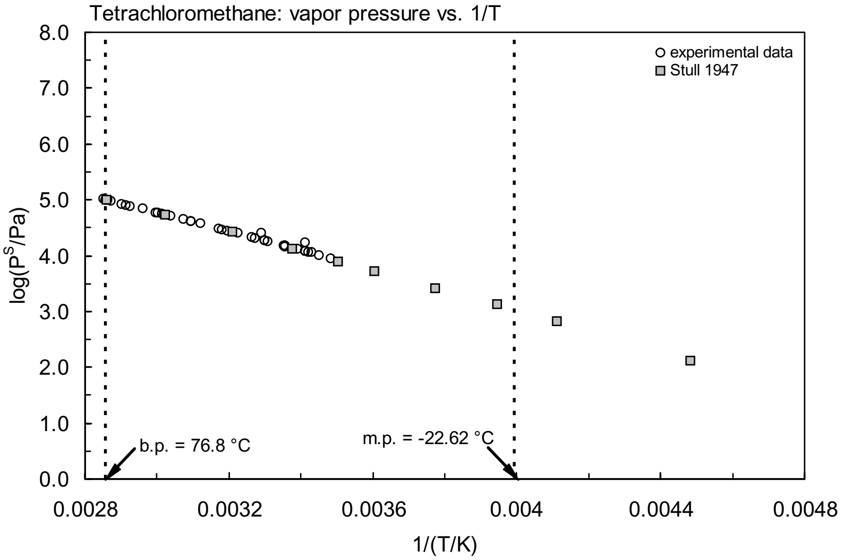


FIGURE 5.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.3
Reported Henry's law constants of tetrachloromethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)
$\ln H = A - B/(T/K)$ (4) $\log H = A - B/(T/K)$ (4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

1.

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancréde & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.0	751.6	10.0	1337.5	10	1500	25	2875
1.3	752.2	17.5	2138	15	1935	26.5	2666
11.0	1312	24.8	3080	20	2351	27.4	3248
13.0	1568	34.6	4661	25	2989	28.9	3315
21.0	2335			30	3830	28.9	3466
22.0	2406	eq. 4	H/(atm m³/mol)			29.7	3525
27.1	2866	A	11.29	eq. 4	H/(atm m³/mol)	29.9	3527
25	2797	B	4411	A	9.739	33.3	4713
				B	3951	35.6	4390
eq. 3	k_H/atm					38.3	5334
A	22.22					40	5546
B	4438					44.7	5416
						45	6993
						47.2	7484
						eq. 1	K_{AW}
						A	5.569
						B	1639

(*Continued*)

TABLE 5.1.1.4.3 (*Continued*)

2.

Tse et al. 1992		Wright et al. 1992		Hansen et al. 1993		Dewulf et al. 1995	
activity coefficient		activity coefficient		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
20	2067	20	2646	27.6	3133	2.0	835
30	3415	35	4550	35.0	4550	6.0	912
35	3871	50	6624	45.0	6343	10.0	1055
40	4580					18.2	1926
				eq. 4	H/(kPa m³/mol)	25.0	2598
				A	13.0		
				B	3553	eq. 1	K_{AW}
						A	13.722
						B	4073

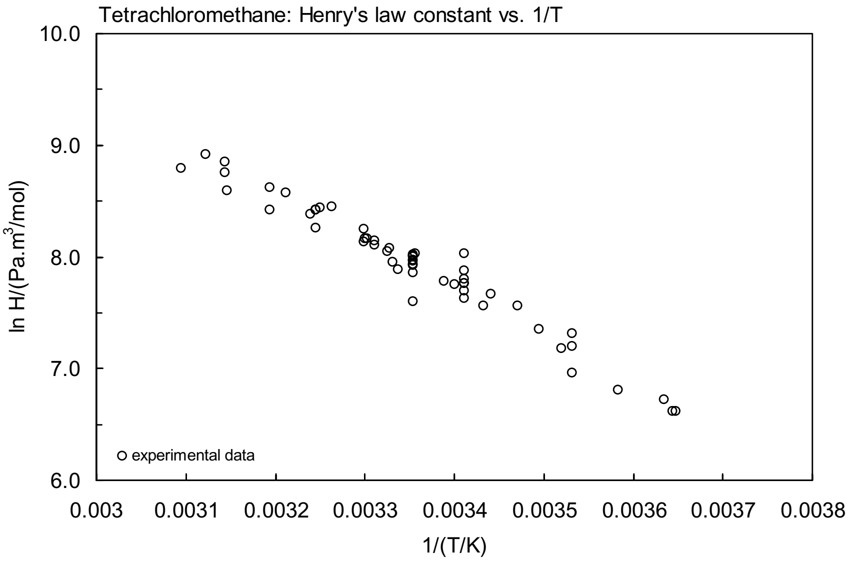


FIGURE 5.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.4
Reported octanol-water partition coefficients of tetrachloromethane at various temperatures

Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		EPICS-GC	
t/°C	log K_{OW}	t/°C	log K_{OW}
25	2.73	2.2	2.39
35	2.74	6.0	2.38
50	2.73	10.0	2.50
		14.1	2.44
		18.7	2.47
		24.8	2.38
		change in enthalpy: $\Delta H_{OW}/(\text{kJ mol}^{-1}) = 1.3$ (–12.1 to 14.6) enthalpy of transfer $\Delta H_{oct}/(\text{kJ mol}^{-1}) = -0.5$ (–13.9 to 12.8)	

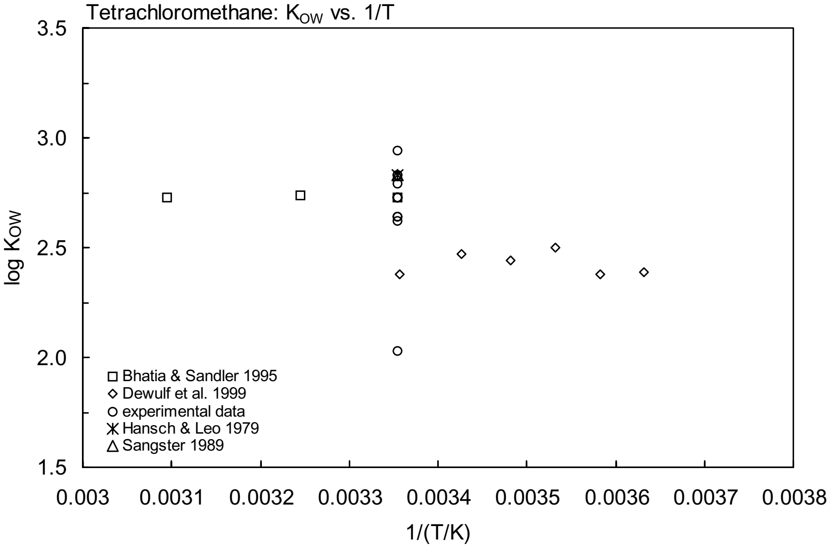
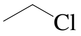


FIGURE 5.1.1.4.4 Logarithm of K_{OW} versus reciprocal temperature for tetrachloromethane.

5.1.1.5 Chloroethane (Ethyl chloride)



Common Name: Ethyl chloride
Synonym: chloroethane, monochloroethane
Chemical Name: chloroethane, ethyl chloride, monochloroethane, hydrochloric ether, muriatic ether
CAS Registry No: 75-00-3
Molecular Formula: C_2H_5Cl, CH_3CH_2Cl
Molecular Weight: 64.514
Melting Point (°C):
–138.4 (Lide 2003)
Boiling Point (°C):
12.30 (McGovern 1943; Weast 1982–83; Dean 1985; Howard 1990; Lide 2003)
Density (g/cm^3 at 20°C):
0.8978 (Weast 1982–83)
0.92390, 0.8960, 0.88981 (0, 20, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
72.0 (calculated-density, Wang et al. 1992)
72.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
27.8, 24.652 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
4.45 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
5735 (12.5°C, shake flask, Führer 1924)
7580 (Seidell 1940)
4500 (0°C, McGovern 1943; Dean 1985)
5710 (20°C, Neely 1976)
5700 (20°C, selected, Dilling 1977)
5678* (20°C, summary of literature data, Horvath 1982)
5740 (20°C, Verschueren 1977, 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are complied at the end of this section):
136630 (data presented in graph, temp range –50 to ~105°C, McGovern 1943)
187000* (extrapolated-Antoine eq. regression, summary of literature data, Stull 1947)
101436* (12.51°C, static method-Hg manometer, measured range –55.88 to 12.51°C, Gordon & Giauque 1948)
160000 (calculated-Antoine eq., Dreisbach 1959)
$\log (P/\text{mmHg}) = 6.94914 - 1012.77/(236.47 + t/°C)$; temp range –50 to 70°C (Antoine eq. for liquid state, Dreisbach 1959)
$\log (P/\text{mmHg}) = 6.94914 - 1012.771/(236.67 + t/°C)$, pressure range of 10 to 1500 mmHg, (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
$\log (P/\text{mmHg}) = [-0.2185 \times 6310.6/(T/K)] + 7.660205$; temp range –89.8 to 180.5°C (Antoine eq., Weast 1972–73)
160000 (calculated-Antoine eq., Boublik et al. 1973)
$\log (P/\text{mmHg}) = 6.98647 - 1030.007/(238.612 + t/°C)$; temp range –55.94 to 12.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
149400 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.11833 - 1033.161/(236.956 + t/°C)$; temp range –55.94 to 12.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.98647 - 1030.01/(238.61 + t/°C)$; temp range –56 to 12.2°C (Antoine eq., Dean 1985, 1992)
159880 (selected, Riddick et al. 1986)
$\log (P/\text{kPa}) = 6.09088 - 1020.63/(237.57 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
160000 (calculated-Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.07404 - 1012.771/(-36.48 + T/K)$; temp range 207–305 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.14258 - 1053.998/(-30.686 + T/K)$; temp range 285–344 K (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.4495 - 1248.788/(-3.798 + T/K)$; temp range: 334–413 K (Antoine eq.-III, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.70739 - 1465.734/(29.696 + T/K)$; temp range 403–460 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = 28.3448 - 2.0788 \times 10^3/(T/K) - 7.5387 \cdot \log (T/K) - 1.6384 \times 10^{-11} \cdot (T/K) + 4.055 \times 10^{-6} \cdot (T/K)^2$; temp range 137–460 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

860 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
1140 (calculated, Dilling 1977)
1145 (calculated-P/C, Mackay & Shiu 1981,1990)
1125* (24.8°C, EPICS-GC/FID, measured range 10.3–34.6°C, Gossett 1987)
$\ln [H/(\text{atm m}^3/\text{mol})] = 5.974 - 3120/(T/K)$; temp range: 10.3–34.6°C (EPICS measurements, Gossett 1987)
1226* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 4.265 - 2580/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
1270 (calculated-QSAR, Nirmalakhandan & Speece 1988)
942 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
701 (computed value, Yaws et al. 1991)
1019 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 3.406 - 1110/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

1.54 (Leo et al. 1971)
1.39 (calculated-π substituent const., Hansch et al. 1968; Hansch & Leo 1979)
1.43 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1987)
1.43 (recommended, Sangster 1989, 1993)
1.43 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

0.86, 0.67 (estimated-K_{OW}, S, Lyman et al. 1982; quoted, Howard et al. 1990)
0.99 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

2.16, 1.52 (estimated-K_{OW}, S, Lyman et al. 1982; quoted, Howard 1990)
1.17 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.40 (soil, selected, Jury et al. 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization: estimated experimental $t_{½}$ = 21 min for 1 mg/L to evaporate from aqueous solution stirred at 200 rpm in an open container of depth 65 mm at 25°C (Dilling et al. 1975);
Evaporation $t_{½}$(exptl) = 23.1 min, $t_{½}$(calc) = 0.5 min, 16.7 min from water (Dilling 1977);
volatilization $t_{½}$ = 2.5 h from a model river of 1 m deep, based on Henry's law constant (Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2}$ = 5.6, 1.1, and 4.5 d from representative pond, river and lake were estimated based on oxygen reaeration ratio of 0.645 (Mabey et al. 1982; quoted, Howard 1990);

$t_{1/2}$ = 30 d for volatilization loss from soil (Jury et al. 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = (3.9 \pm 0.7) \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at 296 K and the calculated lifetime of about 2.6×10^8 s or 30 d (discharge flow-laser magnetic resonance, Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980)

$k_{OH} = (2.37 \pm 0.32) \times 10^9$ $cm^3\ mol^{-1}\ s^{-1}$ or $(3.94 \pm 0.53) \times 10^{-13}$ $cm^3\ molecule^{-1}\ s^{-1}$ at 297 K (flash photolysis-resonance fluorescence, Paraskevopoulos et al. 1978)

$k_{OH} = 2.3 \times 10^{11}$ $cm^3\ mol^{-1}\ s^{-1}$, estimated at 300 K (Lyman 1982)

$k << 360\ M^{-1}\ h^{-1}$ for singlet oxygen and $k << 1\ M^{-1}\ h^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{O3} = 2.0 \times 10^{-23}$ $cm^3 \cdot molecule^{-1}\ s^{-1}$ at 298 K, measured range 298–323 K (quoted, Atkinson & Carter 1984)

photooxidation half-life of 160–1604 h, based on measured rate constants for the reaction with OH radical in air (Atkinson 1985; quoted, Howard 1990; Howard et al. 1991)

$k_{OH} = 3.9 \times 10^{-13}$ $cm^3\ molecule^{-1}\ s^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}* = (4.08 \pm 0.31) \times 10^{-13}$ $cm^3\ molecule^{-1}\ s^{-1}$ at 294.8 K, measured range 294.8–788.7 K (laser photolysis/laser induced fluorescence, Kasner et al. 1990)

Hydrolysis: $k = 2.0 \times 10^{-7}\ s^{-1}$ was estimated for reaction at pH 7 and 25°C with a maximum $t_{1/2}$ = 40 d (Radding et al. 1977; quoted, Callahan et al. 1979; Mabey et al. 1982);

$k = 2.10 \times 10^{-7}\ s^{-1}$ with $t_{1/2}$ = 38 day at 25°C and pH 7 (Mabey & Mill 1978)

estimated $t_{1/2}$ = 38 d at 25°C was based on an exptl $t_{1/2}$ = 1.68 h at 100°C with ethanol and HCl being the hydrolysis product (Mabey & Mill 1978; quoted, Haque et al. 1980; Howard 1990; Howard et al. 1991);

$k = 4.5 \times 10^{-5}\ h^{-1}$ at pH 7 and 25°C with a calculated $t_{1/2}$ = 1.8 yr (Jeffers et al. 1989; quoted, Ellington 1989);

abiotic hydrolysis or dehydrohalogenation $t_{1/2}$ = 1.3 month (Olsen & Davis 1990).

Biodegradation:

$t_{1/2}$(aq. aerobic) = 168–672 h, based on aqueous aerobic screening test data for 1-chloropropane and 1-chlorobutane (Gerhold & Malaney 1966; quoted, Howard et al. 1991)

$t_{1/2}$(aq. anaerobic) = 672–2688 h, based on estimated unacclimated aqueous aerobic half-life (Howard et al. 1991)

$k = 0.02\ yr^{-1}$ with $t_{1/2}$ = 10 d and $k = 0.001\ yr^{-1}$ with $t_{1/2}$ = 700 d (Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetime of about 2.6×10^8 s or 30 d (Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980);

$t_{1/2}$ = 160–1604 h, based on photooxidation half-life in air from measured rate constants for the gas phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 0.04 yr (Nimitz & Skaggs 1992).

Surface water: $t_{1/2}$ = 168–672 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2}$ = 336–1344 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 10–50 d (Ryan et al. 1988);

$t_{1/2}$ = 30 d, volatilization loss from soil (Jury et al. 1990);

$t_{1/2}$ = 168–672 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2}$ = 10–50 d, subject to plant uptake by soil through volatilization (Ryan et al. 1988).

TABLE 5.1.1.5.1
Reported aqueous solubilities and vapor pressures of chloroethane at various temperatures

$$S/(\text{wt\%}) = 0.5842 - 1.6863 \times 10^{-3}\cdot(t/°C) + 9.3949 \times 10^{-5}\cdot(t/°C)^2 - 2.5316 \times 10^{-6}\cdot(t/°C)^3 \quad (1)$$

Aqueous solubility		Vapor pressure			
Horvath 1982		Stull 1947		Gordon & Giauque 1948	
summary of literature data		summary of literature data		static method-Hg manometer	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
0	5842	–89.8	133.3	–55.88	2993
10	5742	–73.9	666.6	–43.64	6726
20	5678	–65.8	1333	–35.44	10992
		–56.8	2666	–28.085	16549
eq. 1	S/wt%	–47.0	5333	–19.99	25119
		–40.6	7999	–13.48	34379
		–32.0	13332	–7.64	44878
		–18.6	26664	–1.878	57621
		–3.90	53329	3.448	17859
		12.4	101325	6.481	81100
				10.48	94708
		mp/°C	–139	12.51	101436
				mp/K =	134.80
				bp/K =	285.37
				$\log P = A - B/(T/K) - C\cdot(T/K) + D\cdot(T/K)^2$	
					P/cmHg
				A	10.54417
				B	1777.378
				C	0.0115789
				D	1.06734×10^5
				$\Delta H_{fus}/(\text{kJ mol}^{-1}) = 4.452$	
				$\Delta H_V/(\text{kJ mol}^{-1}) = 24.65$	
					at 285.37 K

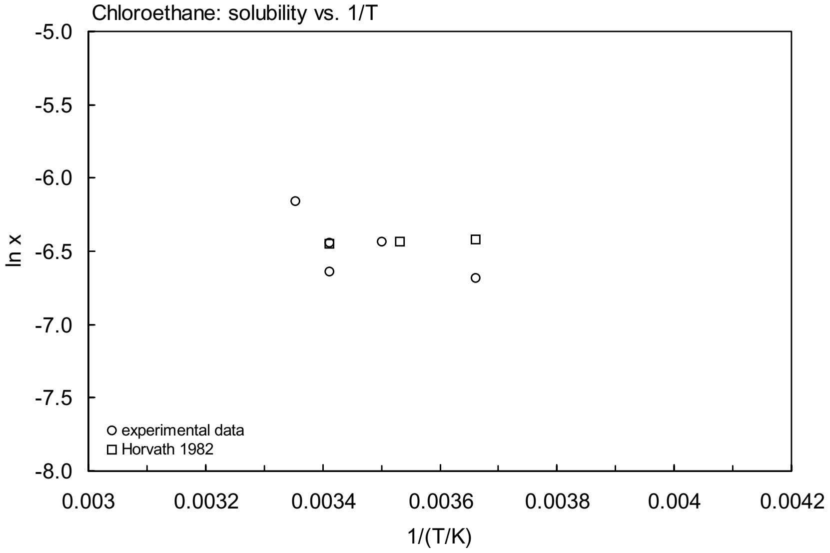


FIGURE 5.1.1.5.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for chloroethane.

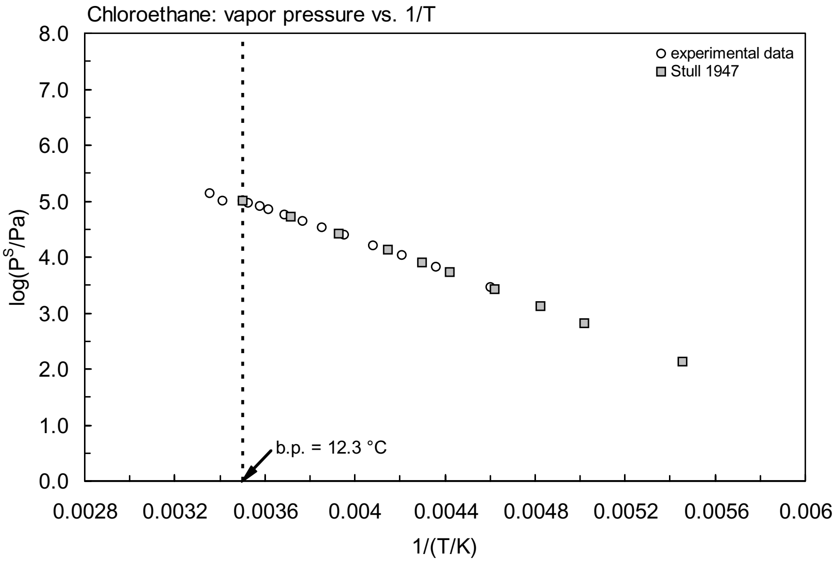


FIGURE 5.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for chloroethane.

TABLE 5.1.1.5.2
Reported Henry's law constants of chloroethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)		$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)		$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)		$\ln [H/(\text{atm·m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B·(T/K) + C·(T/K)^2$	(5)			

Gossett 1987		Ashworth et al. 1988	
EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
10.3	660	10	769
17.5	857.2	15	970.7
24.8	1125	20	1115
34.6	1571	25	1226
		30	1449
eq. 4a	H/(atm m³/mol)		
A	7.385	eq. 4a	H/(atm m³/mol)
B	3286	A	4.265
		B	2580

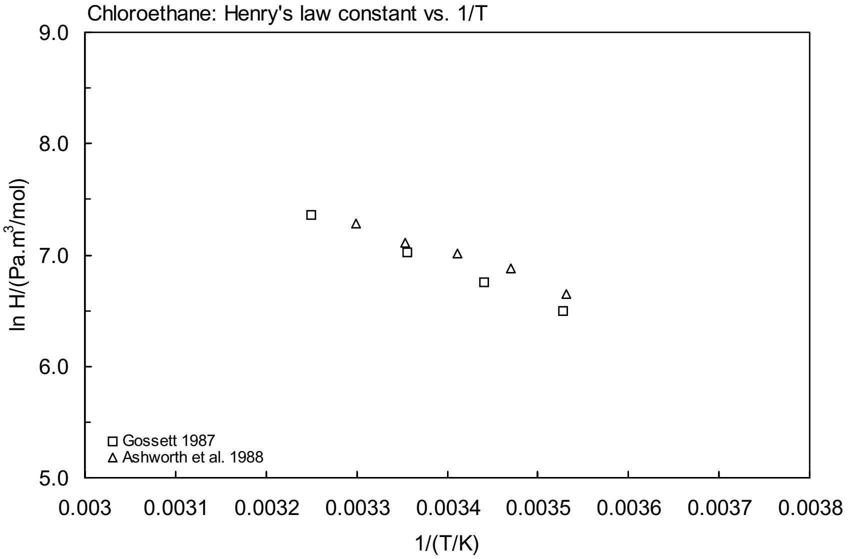
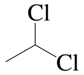


FIGURE 5.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for chloroethane.

5.1.1.6 1,1-Dichloroethane



Common Name: 1,1-Dichloroethane
Synonym: ethylidene chloride, ethylidene dichloride
Chemical Name: 1,1-dichloroethane
CAS Registry No: 75-34-3
Molecular Formula: $C_2H_4Cl_2$, CH_3CHCl_2
Molecular Weight: 98.959
Melting Point (°C):
–96.9 (Lide 2003)
Boiling Point (°C):
57.3 (Weast 1982–83, Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 20°C):
1.1757 (Dreisbach 1961; Horvath 1982; Weast 1982–83; Dean 1985)
1.1755, 1.1679 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
84.0 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)
93.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
30.62, 28.6 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
7.87 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
5500* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
5060 (shake flask-interferometer, Gross 1929; quoted, Horvath 1982)
5555 (volumetric method, Wright & Schaffer 1932)
5060* (20°C, shake flask, measured range 0–50°C, Van Arkel & Vles 1936)
5060 (Seidell 1941)
4800* (shake flask, measured range 10–70°C, Walraevens et al. 1974)
$\log [S/(mol/L)] = 2070/(T/K) - 15.116 + 0.0230\cdot(T/K)$, temp range 10–70°C, Walraevens et al. 1974
5100 (literature average, Dilling 1977, 1982)
4767* (summary of literature data, temp range 0–80°C, Horvath 1982)
4834 (30°C, headspace-GC analysis. McNally & Grob 1983)
4589 (30°C, headspace-GC analysis, McNally & Grob 1984)
5030 (20°C, selected, Riddick et al. 1986)
5090, 4910, 5090 (20, 35, 50°C, infinite dilution activity coeff. γ^∞-GC, Barr & Newsham 1987)
4842, 4984 (predicted-MCI χ and polarizability, Nirmalakhandan & Speece 1988)
5240, 5317, 5406 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
6560, 7300, 8085 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
4998, 4434, 5236 (20, 35, 45°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
5196* (20°C, activity coeff. by inert air stripping-GC, measured range 10–50°C, Hovorka & Dohnal 1997)
5040* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
$S/(wt\%) = 9.4136 - 5.7249 \times 10^{-2}\cdot(T/K) + 9.17839 \times 10^{-5}\cdot(T/K)^2$, temp range 273–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
24300, 37000 (20°C, 30°C, Rex 1906)

30000* (Antoine eq. regression, temp range –60.7 to 57.4°C, Stull 1947)
22001* (17.62°C, static-Hg manometer, measured range –38.76 to 17.62°C, Li & Pitzer 1956)
30400 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6/9853 – 1171.42/(228.12 + t/°C); temp range –15 to 82°C (Antoine eq. for liquid state, Dreisbach 1961)
26000 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 7288.0/(T/K)] + 7.629952; temp range –60.7 to 261.5°C (Antoine eq., Weast 1972–73)
30260 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 6.97702 – 1174.022/(229.06 + t/°C); temp range –38.8 to 17.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
30260 (Boublik et al. 1984)
log (P/kPa) = 6.10983 – 1177.636/(229.409 + t/°C); temp range –38.8 to 17.5°C(Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9971 – 1174.02/(229.08 + t/°C); temp range –39 to 16°C (Antoine eq., Dean 1985, 1992)
30360 (selected, Riddick et al. 1986)
log (P/kPa) = 6.16780 – 1201.05/(231.27 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
30360 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.1102 – 1171.42/(–45.03 + T/K); temp range 258–365 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.14443 –1216.12/(–36.569 + T/K); temp range 323–535 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.22839 – 1288.092/(–24.381 + T/K); temp range 363–535 K (Antoine eq.-III, Stephenson & Malanowski 1987)
24440, 37240 54990 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 33.380 – 2.6102 × 10^3/(T/K) – 9.1336·log (T/K) – 2.8838 × 10^{-11}·(T/K) + 3.7323 × 10^{-6}·$(T/K)^2$; temp range 176–523 K (vapor pressure eq., Yaws 1994)
log (P/kPa) = 6.110022 – 1171.420/(T/K – 45.03) (from database of CDATA 1991, Hovorka & Dohnal 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
595 (calculated-1/K_{AW} (C_W/C_A) reported as exptl., Hine & Mookerjee 1975)
595 (calculated-P/C, Dilling 1977)
log (k_H/atm) = 8.87 – 1902.37/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)
569* (EPICS-GC/FID, measured range 9.6–34.6°C, Gossett 1987)
ln [H/(atm m^3/mol)] = 9.637 – 4128/(T/K); temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)
552 (gas stripping-GC, Warner et al. 1987)
633* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 5.484 – 3137/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
436 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
584 (calculated-P/C, Mackay & Shiu 1990)
595 (computed value, Yaws et al. 1991)
436 (20°C, quoted from Gossett 1987, Tse et al. 1992)
466, 709, 1034 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
477, 995, 1226 (20, 35, 45°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
588, 1125, 1844 (25, 35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
511* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)
246, 627 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
ln K_{AW} = –3975/(T/K) + 0.00768·Z + 11.727; with Z salinity 0–35.5‰, temp range: 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)
526 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
466* (20°C, equilibrium air stripping-GC, measured range 10–50°C, Hovorka & Dohnal 1997)
500 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 4.416 – 1498/(T/K) (summary of literature data, Staudinger & Roberts 2001)

592* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
ln K_{AW} = 10.09 – 3447.7/(T/K); temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

1.79	(shake flask-GC, Hansch et al. 1975, Hansch & Leo 1987)
1.92	(Hansch & Leo 1979)
1.79	(recommended, Sangster 1993)
1.89	(calculated-activity coefficients, Tse & Sandler 1994)
1.82*	(infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
1.79	(recommended, Hansch et al. 1995)
1.75*	(24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

2.41	(calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

1.20	(estimated-S, Lyman et al. 1982)
1.28	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

1.60	(estimated-S, Lyman et al. 1982)
1.48	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.66	(soil, selected, Jury et al. 1990)

1.43, 1.46, 1.43, 1.48, 1.50, 1.49, 1.55 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon f_{OC} = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization: estimated experimental $t_{½}$ = 22 min for initial concentration of 1.0 mg/L when stirred at 200 rpm in water at approx. 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation $t_{½}$(exptl) = 32.2 min, $t_{½}$(calc) = 0.98 min, 21.2 min from water (Dilling 1977);

$t_{½}$ = 6–9 d in a typical pond, $t_{½}$ = 5–8 d in a typical lake, and $t_{½}$ = 24–32 h in a typical river (Smith et al. 1980; quoted, Howard 1990);

ratio of rate of evaporation to that of oxygen reaeration: measured value of 0.57 compared to that predicted value of 0.47 (Smith et al. 1980);

$t_{½}$ = 45 d for the volatilization loss from soil (Jury et al. 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (2.6 ± 0.6) × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow-laser magnetic resonance, Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980; Howard 1990)

k_{OH} = 2.6 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1}, residence time of 44 d, loss of 2.3% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

k_{OH} < 1.6 × 10^{11} cm^3 mol^{-1} s^{-1} for the reaction with OH radical at 300 K (Lyman 1982)

k << 360 M^{-1} h^{-1} for singlet oxygen and 1.0 M^{-1} h^{-1} for peroxy radical both at 25°C (Mabey et al. 1982; quoted, Ma et al. 1990)

photooxidation $t_{½}$ = 247–2468 h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis: k = 1.15 × 10^{-7} M^{-1} h^{-1} for neutral process by analogy to dichloromethane (Mabey et al. 1982);

k = 1.29 × 10^{-6} h^{-1} at pH 7 and 25°C with calculated $t_{½}$ = 61 yr (Jeffers et al. 1989; quoted, Ellington 1989).

Biodegradation: $t_{½}$(aq. aerobic) = 768–3696 h, based on estimated methane acclimated soil grab sample data (Henson et al. 1989; quoted, Howard et al. 1991) and sub-soil grab sample data from a ground water aquifer

(Wilson et al. 1983; quoted, Howard et al. 1991); $t_{1/2}$(aq. anaerobic) = 3072–14784 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2}$ > 60 d (Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$: = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetime of 1.5 months based on reaction with OH radical (Callahan et al. 1979; Altshuller 1980; Howard 1990);

residence time of 44 d, loss of 2.3% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2}$ = 247–2468 h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 0.02 yr (Nimitz & Skaggs 1992).

Surface water: $t_{1/2}$ = 768–3696 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2}$ = 1344–8640 h, based on estimated aqueous aerobic biodegradation half-life and sub-soil grab sample data from a groundwater aquifer (Wilson et al. 1983; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 10–50 d (Ryan et al. 1988);

$t_{1/2}$: = 768–3696 h, based on methane acclimated soil grab sample data (Henson et al. 1989; quoted, Howard et al. 1991) and sub-soil grab sample data from a groundwater aquifer (Wilson et al. 1983; quoted, Howard et al. 1991);

$t_{1/2}$ = 45 d, volatilization loss from soil (Jury et al. 1990).

Biota: $t_{1/2}$ < 2 d of elimination from whole body of bluegill sunfish (USEPA 1980; quoted, Howard 1990);

$t_{1/2}$ = 10–50 d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.6.1
Reported aqueous solubilities of 1,1-dichloroethane at various temperatures

$$S/(\text{wt\%}) = 0.5826 - 7.8236 \times 10^{-3}\cdot(t/°C) + 1.5268 \times 10^{-4}\cdot(t/°C)^2 - 3.6609 \times 10^{-7}\cdot(t/°C)^3 \quad (1)$$

$$S/(\text{wt\%}) = 9.4136 - 5.7249 \times 10^{-2}\cdot(T/K) + 9.17839 \times 10^{-5}\cdot(T/K)^2 \quad (2)$$

1.

Rex 1906		Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982	
volumetric method		shake flask		shake flask-GC		summary of literature data	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
0	6560	0	5940	10	5030	0	5826
10	5950	20	5060	20	4830	10	5193
20	5500	35	4820	25	4800	20	4843
30	5400	50	5190	30	4810	25	4766
				40	4960	30	4754
				50	5280	40	4905
				60	5790	50	5274
				70	8520	60	5838
				80	7510	70	6575
						80	7465
						eq.1	S/wt%

(*Continued*)

TABLE 5.1.1.6.1 (*Continued*)

2.

Barr & Newsham 1987		**Wright et al. 1992**		**Hovorka & Dohnal 1997**		**Horvath & Getzen 1999a**	
infinite dilution activity coeff.		**activity coefficient**		**activity coefficient**		**recommended, IUPAC-NIST**	
t/°C	**$S/g·m^{-3}$**	**t/°C**	**$S/g·m^{-3}$**	**t/°C**	**$S/g·m^{-3}$**	**t/°C**	**$S/g·m^{-3}$**
20	5090	20	4998	10	5627	0	6240
35	4910	35	4434	20	5196	5	5910
50	5090	45	5236	30	5236	10	5620
				35	5266	15	5380
				40	5395	20	5190
				45	5576	25	5040
		Tse et al. 1992		50	5812	30	4930
		activity coefficient				35	4880
		t/°C	**$S/g·m^{-3}$**			40	4870
						45	4900
		20	5240			50	4980
		30	5317				
		40	5406			eq. 2	S/wt%
						temp range 273–323 K	

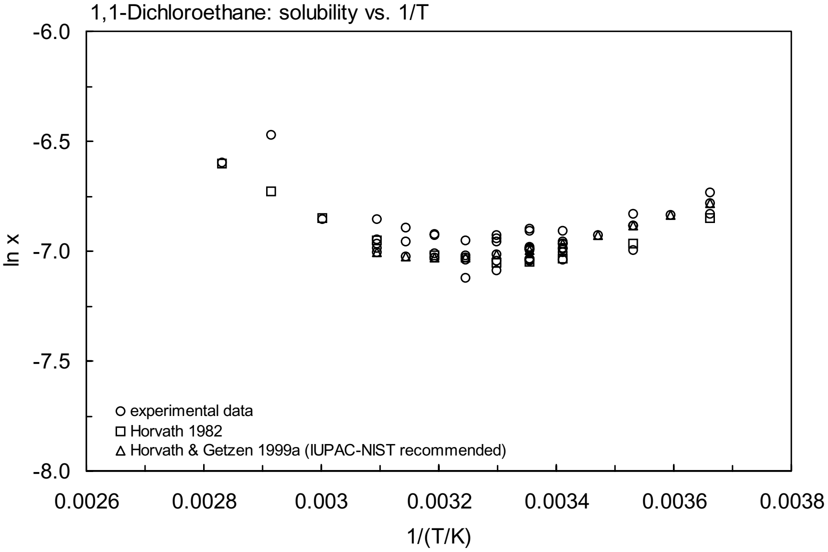


FIGURE 5.1.1.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.2
Reported vapor pressures of 1,1-dichloroethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log (T/K)$ (4)

Stull 1947		**Li & Pitzer 1956**			
summary of literature data		**static-Hg manometer**			
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
–60.7	133.3	–38.76	858.6	11.34	16536
–41.9	666.6	–29.61	1649	17.50	21876
–32.3	1333	–20.21	3020	17.62	22001
–21.9	2666	–19.18	3234		
–10.2	5333	–18.16	3301	mp/°C	–96.98
–2.90	7999	–17.69	3517		
7.20	13332	–16.82	3716	eq. 2	P/cmHg
22.4	26664	–12.61	4772	A	6.1560
39.8	53329	–12.20	4869	B	1258.1
57.4	101325	–2.23	8425	C	26.0
		1.18	10077	$\Delta H_{fus}/(kJ\ mol^{-1}) = 7.87$	
mp/°C	–96.7	11.10	16333	$\Delta H_V/(kJ\ mol^{-1}) = 31.02$	

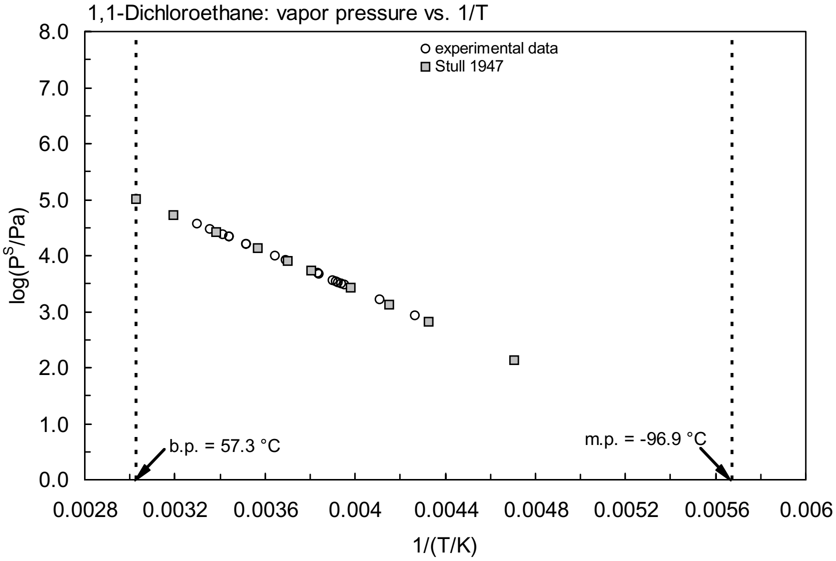


FIGURE 5.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.3
Reported Henry's law constants of 1,1-dichloroethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)

$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)

$\ln (k_H/atm) = A - B/(T/K)$ (3)

$\ln H = A - B/(T/K)$ (4) $\log H = A - B/(T/K)$ (4a)

$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

1.

Gossett 1987		Ashworth et al. 1988		Tse et al. 1992		Wright et al. 1992	
EPICS-GC		EPICS-GC		activity coefficient		activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
9.6	251.3	10	373	20	466	20	477
17.5	394.2	15	460	30	709	35	995
24.8	569.4	20	570	40	1034	45	1226
34.6	820.7	25	631				
		30	786				
eq. 4	H/(atm m³/mol)						
A	8.637	eq. 4	H/(atm m³/mol)				
B	4128	A	5.484				
		B	3137				

2.

Bhatia & Sandler 1995		Dewulf et al. 1995		Hovorka & Dohnal 1997		Görgényi et al. 2002	
activity coefficient		EPICS-GC		equilibrium air stripping-GC		EPICS-SPME method	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
25	588	2	152.1	10	273	2	174
35	1125	6	195.2	20	466	6	240.4
50	1844	10	194.7	30	692	10	283.9
		18.2	378.2	35	851	18	452.4
		25	510.6	40	1010	25	592.4
				45	1172	30	760.9
		eq. 1	K_{AW}	50	1338	40	1059
		A	11.727			50	1472
		B	3975			60	1907
						eq. 1	K_{AW}
						A	10.09
						B	3447.7

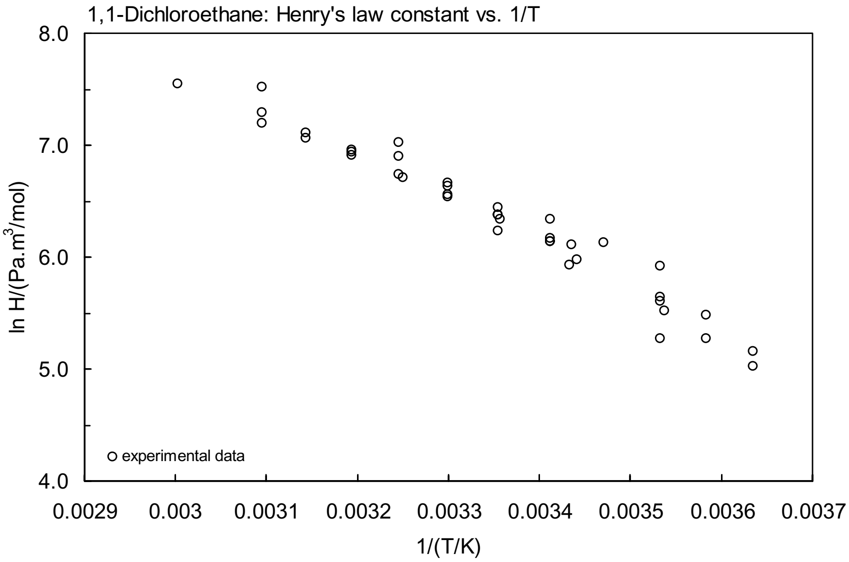


FIGURE 5.1.1.6.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.4
Reported octanol-water partition coefficients of 1,1-dichloroethane at various temperatures

Bhatia & Sandler 1995		DeWulf et al. 1999	
relative GC-RT technique		EPICS-GC	
t/°C	log K_{OW}	t/°C	log K_{OW}
25	1.82	2.2	1.70
35	1.66	4.0	1.69
50	1.68	10.0	1.74
		14.1	1.73
		18.7	1.78
		24.8	1.75
		change in enthalpy: $\Delta H_{OW}/(kJ\ mol^{-1}) = 5.2$ (0.0 to 10.4) enthalpy of transfer $\Delta H_{oct}/(kJ\ mol^{-1}) = 2.5$ (–2.7 to 7.7)	

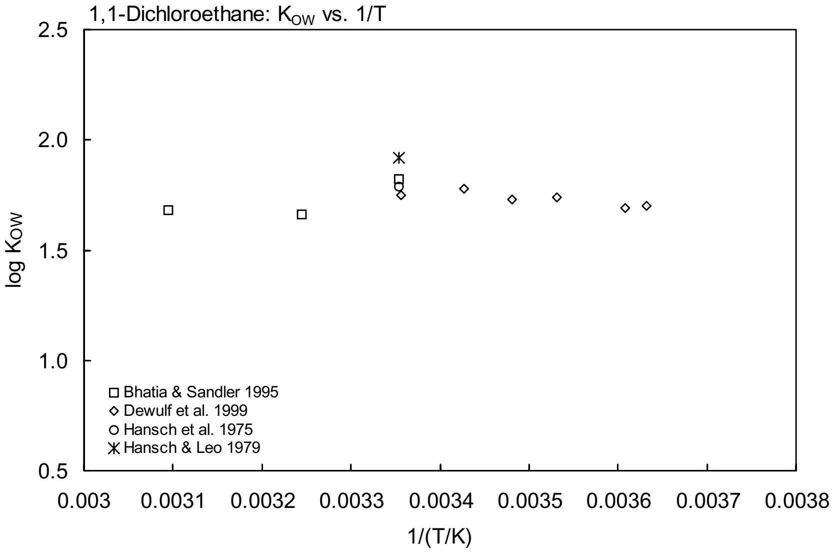
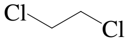


FIGURE 5.1.1.6.4 Logarithm of K_{OW} versus reciprocal temperature for 1,1-dichloroethane.

5.1.1.7 1,2-Dichloroethane



Common Name: 1,2-Dichloroethane
Synonym: ethylene chloride, ethylene dichloride, glycol dichloride, sym-dichloroethane, Dutch oil, EDC
Chemical Name: 1,2-dichloroethane
CAS Registry No: 107-06-2
Molecular Formula: $C_2H_4Cl_2$, CH_2ClCH_2Cl
Molecular Weight: 98.959
Melting Point (°C):
  –35.7 (Lide 2003)
Boiling Point (°C):
  85.3 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.2531, 1.2458 (20°C, 25°C, Dreisbach 1959; Dean 1985)
  1.25209, 1.24637 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
  78.0 (calculated-density, Wang et al. 1992)
  93.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  35.15, 32.02 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  1.982 (calculated, Dreisbach 1959)
  2.112 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  8690* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
  8650 (shake flask-interferometer, Gross 1929)
  8720, 9000 (15°C, 30°C, shake flask-interferometer, Gross & Saylor 1931)
  8696 (volumetric method, Wright & Schaffer 1932)
  8490* (20°C, shake flask, measured range 0–56°C, Van Arkel & Vles 1936)
  8620 (Seidell 1940)
  8400 (data presented in graph, temp range 0–70°C, McGovern 1943; Horvath 1982)
  8610* (shake flask-GC, temp range 0–80°C, Walraevens et al. 1974)
  $\log [S/(mol/L)] = 2070/(T/K) - 15.369 + 0.0247\cdot(T/K)$; temp range 0–80°C (Walraevens et al. 1974)
  8800 (shake flask-GC, McConnell et al. 1975)
  8800 (20°C, Pearson & McConnell 1975)
  8570, 8390, 10250 (3, 20, 34°C, shake flask-GC/ECD, Chiou & Freed 1977)
  8450 (shake flask-GC, Chiou et al. 1979)
  8630 (20°C, recommended, Sørensen & Arit 1979)
  7987 (shake flask-LSC, Banerjee et al. 1980)
  10600 (shake flask-titration, Coca & Diza 1980)
  11000 (shake flask-titration/turbidity, Coca et al. 1980)
  8000 (shake flask-LSC, Veith et al. 1980)
  8608* (summary of literature data, temp range 0–80°C, Horvath 1982)
  3506 (30°C, shake flask-headspace-GC, McNally & Grob 1984)
  8044 (calculated-UNIFAC activity coeff., Banerjee 1985)
  8100 (Dean 1985, Riddick et al. 1986)
  8782, 9102, 9960 (20, 35, 50°C, infinite dilution activity coeff. γ^∞-GC, Barr & Newsham 1987)
  7200* (19.7°C, shake flask-GC/TC, measured range 0–80°C, Stephenson 1992)
  8500, 9013, 9163 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)

7809, 8727, 9209 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
9400, 9209, 9835 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
6537 (20°C, activity coeff. γ^∞ by inert air stripping-GC, Hovorka & Dohnal 1997)
8600* (recommended, temp range 0–100°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 17.9147 – 0.11684·(T/K) + 2.0003 × 10^{-4}·$(T/K)^2$, temp range 273–373 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)404

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
8130, 12980 (20°C, 30°C, Rex 1906)
10519* (isoteniscope method, measured range –30.82 to 99.4°C, Pearce & Peters 1929)
log (P/mmHg) = 128.756 – 4481.12/(T/K) – 52.3092·log (T/K) + 0.07153·(T/K) – 4.1847 × 10^{-5}·$(T/K)^2$; temp range 243–363 K (isoteniscope method, Pearce & Peters 1929)
10660 (McGovern 1943)
10740* (interpolated-Antoine eq., regression, temp range –30.8 to 99.4°C, Stull 1947)
10700 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 7.18431 – 1358.5/(252.0 + t/°C); temp range 6–161°C (Antoine eq. for liquid state, Dreisbach 1959)
10150 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 7950.7/(T/K)] + 7.708405; temp range –44.5 to 285°C (Antoine eq., Weast 1972–73)
10500 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.0253 – 1271.254/(222.927 + t/°C); temp range –30.82 to 99.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
8520 (McConnell et al. 1975)
8400 (Pearson & McConnell 1975)
13282*, 65145 (30, 70°C, vapor-liquid equilibrium VLE data, measured range 28.75–85.54°C, Gutsche & Knapp 1982)
ln (P/kPa) = 14.142372 – 2896.480/[(T/K) – 52.506]; temp range 301.9–357.69 K (vapor-liquid equilibrium VLE data, Gutsche & Knapp 1982)
10500 (Boublik et al. 1984)
log (P/kPa) = 6.16284 – 1278.323/(223.694 + t/°C); temp range –30.82 to 99.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.13975 – 1256.68/(220.504 + t/°C); temp range 28.75–84.54°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 7.0253 – 1271.3/(222.9 + t/°C); temp range –31 to 99°C (Antoine eq., Dean 1985, 1992)
11110 (selected, Riddick et al. 1986)
11100 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.07712 – 1247.8/(–50.15 + T/K); temp range 279–434 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.53278 – 1599.07/(–3.303 + T/K); temp range 356–558 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.07287 – 1245.488/(–50.392 + T/K); temp range 279–374 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.40918 – 1505.414/(–14.406 + T/K); temp range 368–524 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.5198 – 2129.577/(T/K); temp range 523–561 K (Antoine eq.-V, Stephenson & Malanowski 1987)
10462 (resistance measurements-Antoine eq., Foco et al. 1992)
8270, 13320, 16720 (20, 30, 35°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 48.4226 – 3.1803 × 10^3/(T/K) – 15.37·log (T/K) + 7.2935 × 10^{-3}·(T/K) + 2.6844 × 10^{-14}·$(T/K)^2$; temp range 237–561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.1 (exptl., 1/K_{AW} (C_W/C_A), Hine & Mookerjee 1975)
92.3 (calculated-C_W/C_A, McConnell et al. 1975; Peason & McConnell 1975)

99.0, 123.9 (exptl., calculated-P/C, Dilling 1977)
111.3 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
174* (27.0°C, equilibrium cell-concn ratio-GC/FID, measured range 1.0–27.0°C, Leighton & Calo 1981)
$\ln (k_H/\text{atm}) = 18.51 - 3482/(T/K)$; temp range:1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
110 (recommended, Mackay & Shiu 1981)
111.5 (gas stripping-GC, Warner et al. 1987)
143* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = -1.371 - 1522/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
92.0 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
70.8 (computed value, Yaws et al. 1991)
101, 152, 182 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
110, 185, 319 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
122.5 (γ^∞ from gas stripping-GC, Li et al. 1993)
5.30, 8.99 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
102.1* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)
55.9, 123 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
$\ln K_{AW} = -4329/(T/K) + 0.00473\cdot Z + 11.377$; with Z salinity 0–35.5‰, temp range: 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)
110 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
95.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1998)
185.2 (EPICS-GC, Ayuttaya et al. 2001)
102 (20°C, selected from reported experimentally determined values, Staudinger & Roberts 2001)
$\log K_{AW} = 4.434 - 1705/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
1.48 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979, 1987)
1.45 (shake flask-LSC, Banerjee et al. 1980; Veith et al. 1980)
1.58, 1.54 (calculated-octanol and water mutual solubility not considered, calculated-octanol and water mutual solubility considered, Arbuckle 1983)
1.44 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
1.48 (recommended, Sangster 1993)
1.55 (calculated-from activity coefficients, Tse & Sandler 1994)
1.51* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
1.48 (recommended, Hansch et al. 1995)
1.46* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
2.78 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
0.30 (bluegill sunfish, Barrows et al. 1980)
0.301 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
0.954 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982; quoted, Ma et al. 1990)
0.30 (bluegill sunfish, Davies & Dobbs; quoted, Sabljic 1987; Ma et al. 1990)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
1.28 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
1.51 (soil, quoted from Chiou et al. 1979, Karickhoff 1981)
1.06, 1.19, 1.48 (estimated-K_{OW}, estimated-S and mp, estimated-S, Karickhoff 1981)
2.18 (estimated-K_{OW}, Lyman et al. 1982;)
1.15 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.09 (BUA 1987; quoted, Brüggemann et al. 1991)

1.34 (soil, selected, Jury et al. 1990)
1.64, 1.645, 1.64, 1.68, 1.70, 1.65, 1.68 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon f_{OC} = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)

Sorption Partition Coefficient, log K_{OM}:
1.28, 1.50 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization: estimated experimental half-life of volatilization from aqueous solution of 1 mg/L to be (28 ± 1) min when stirred at 200 rpm in water at appro. 25°C in an open container (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);
Evaporation $t_{½}$(exptl) = 28.0 min, $t_{½}$(calc) = 4.5 min, 24.5 min from water (Dilling 1977)
rate of evaporation k = 2.4 g m^{-2} s^{-1} (Environment Canada 1984);
$t_{½}$ = 90 d, estimated volatilization loss from soil (Jury et al. 1990).
Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 1.1 ppm/min per gram of catalyst (Ollis 1985)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = (2.2 \pm 0.5) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow-laser magnetic resonance, Howard & Everson 1976b; quoted, Callahan et al. 1979)
$k_{OH} = 0.1 \times 10^9$ M^{-1} s^{-1} and $t_{½}$ = 234 h (Radding et al. 1977; quoted, Callahan et al. 1979)
$k_{OH} = 2.2 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} with residence time of 53 d, loss of 1.9% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$k_{OH} = 1.3 \times 10^{11}$ cm^3 mol^{-1} s^{-1}, estimated, at 300 K (Lyman 1982)
k < 360 M^{-1} h^{-1} for singlet oxygen and k < 1 M^{-1} h^{-1} for peroxy radicals at 25°C(Mabey et al. 1982)
photooxidation $t_{½}$ = 292–2917 h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991)
k(aq.) ≤ 0.05 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21°C, with a $t_{½}$ ≥ 8 d at pH 7 (Yao & Haag 1991).
Hydrolysis:
$k = 5 \times 10^{-13}$ s^{-1} with a max. $t_{½}$ = 50,000 yr at pH 7 and 25°C from experimental data at 100–150°C (Radding et al. 1977; quoted, Callahan et al. 1979);
$k = 1.80 \times 10^{-9}$ h^{-1} for neutral process (Mabey et al. 1982; quoted, Ma et al. 1990)
$t_{½}$(abiotic) or $t_{½}$(dehydrohalogenation) = 50 months (Mabey et al. 1983; quoted, Olsen & Davis 1990)
k(neutral) = .63 yr^{-1} with first-order $t_{½}$ = 1.1 yr (Kollig et al. 1987; quoted, Howard et al. 1991)
$k = 1.1 \times 10^{-6}$ h^{-1} at pH 7 and 25°C with calculated $t_{½}$ = 72 yr (Jeffers et al. 1989; quoted, Ellington 1989; Brüggemann et al. 1991)
$t_{½}$ = 400 d at pH 7 in natural waters (Capel & Larson 1995)
Biodegradation: relatively undegradable (Lyman et al. 1982; quoted, Brüggemann et al. 1991)
$k < 1.4 \times 10^{-5}$ min^{-1} disappearance rate in sediment-water sample, with $t_{½}$ > 35 d (Jafvert & Wolfe 1987)
$t_{½}$(aq. aerobic) = 2400–4320 h, based on unacclimated grab sample of aerobic soil from ground water aquifers and acclimated river die-away rate data (Wilson et al. 1983; Mudder 1981; quoted, Howard et al. 1991)
$t_{½}$(aq. anaerobic) = 9600–17280 h (Howard et al. 1991)
$t_{½}$ > 60 d (Olsen & Davis 1990)
$t_{½}$(aerobic) = 100 d, $t_{½}$(anaerobic) = 400 d in natural waters (Capel & Larson 1995)
Biotransformation: estimated to be 1×10^{-10} mL $cell^{-1}$ h^{-1} for bacteria (Mabey et al. 1982).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: tropospheric $t_{½}$ = 17 wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)
disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
lifetime of 1.7 months at 296 K based on reaction with OH radical (Callahan et al. 1979);

residence time of 53 d, loss of 1.9% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$t_{½}$ = 292–2917 h, based on photooxidation half-life in air from measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 0.09 yr (Nimitz & Skaggs 1992).

Surface water: $t_{½}$ = 2400–4320 h, based on unacclimated grab sample of aerobic soil from ground water aquifers and acclimated river die-away rate data (Wilson et al. 1983; Mudder 1981; quoted, Howard et al. 1991);

$t_{½}$ > 35 d in sediment-water sample (Jafvert & Wolfe 1987)

$t_{½}$(aerobic) = 100 d, $t_{½}$(anaerobic) = 400 d in natural waters (Capel & Larson 1995)

measured rate constant k ≤ 0.05 $M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with $t_{½}$ ≥ 8 d at pH 7 (Yao & Haag 1991).

Ground water: $t_{½}$ = 2400–8640 h, based on unacclimated grab sample of aerobic soil from ground water aquifers and estimated aqueous aerobic biodegradation half-life (Wilson et al. 1983; Howard et al. 1991).

Sediment: $t_{½}$ > 35 d in Bar-H sediment-water sample (Jafvert & Wolfe 1987)

Soil: $t_{½}$ = 10–50 d (Ryan et al. 1988);

$t_{½}$ = 90 d, estimated volatilization loss from soil (Jury et al. 1990);

$t_{½}$ = 2400–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: 1 < $t_{½}$ < 2 d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{½}$ = 10–50 d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.7.1
Reported aqueous solubilities of 1,2-dichloroethane at various temperatures

$$\log [S/(mol/L)] = -A + 2070/(T/K) + B(T/K) \qquad (1)$$

$$S/(wt\%) = 0.888 - 4.0468 \times 10^{-3}\cdot(t/°C) + 9.37388 \times 10^{-5}\cdot(t/°C)^2 + 9.8465 \times 10^{-7}\cdot(t/°C)^3 \qquad (2)$$

$$S/(wt\%) = 17.9147 - 0.11684\cdot(T/K) + 2.0003 \times 10^{-4}\cdot(T/K)^2 \qquad (3)$$

1.

Rex 1906		Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982	
volumetric method		shake flask		shake flask		summary of literature data	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$*	t/°C	$S/g\cdot m^{-3}$
0	9220	0	8370	10	8520	0	8880
10	8650	20	8490	20	8490	10	8579
20	8690	36	8950	25	8610	20	8524
30	8904	56	10300	30	8800	25	8608
				40	9440	30	8775
				50	10460	40	9391
				60	11920	50	10430
				70	13950	60	11951
				80	16720	70	14014
						80	16678
				eq. 1	S/(mol/L)		
				A	15.369	eq. 1	S/wt%
				B	0.0247		

*data calculated by Horvath 1982

Gross & Saylor 1931	
shake flask-IR	
t/°C	$S/g\cdot m^{-3}$
15	8720
30	9000

(Continued)

TABLE 5.1.1.7.1 *(Continued)*

2.

Barr & Newsham 1987		Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
infinite dilution activity coeff.		shake flask-GC		activity coefficient		activity coefficient	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	8782	0	8200	20	8500	20	9400
35	9102	9.3	7700	30	9013	35	9209
50	9960	19.7	7200	40	9163	50	9835
		29.7	8100				
		39.4	9800				
		50.3	10600				
		61.0	10800				
		70.6	11300				
		80.7	10600				

3.

Horvath & Getzen 1999a					
recommended, IUPAC-NIST					
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	9240	40	9410	80	15990
5	8910	45	9890	85	17270
10	8680	50	10460	90	18640
15	8550	55	11130	95	20110
20	8520	60	11900	100	21680
25	8600	65	12780		
30	8770	70	13750	eq. 2	S/wt%
35	9040	75	14820	temp range 273–373 K	

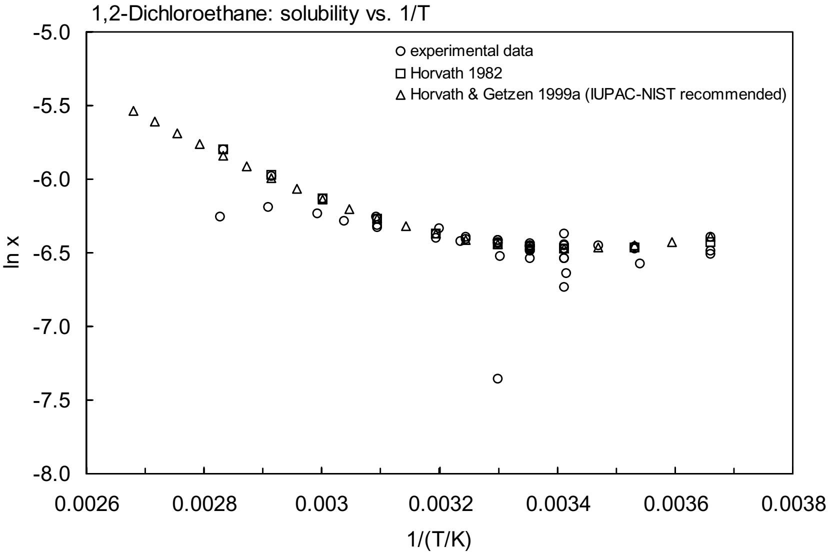


FIGURE 5.1.1.7.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,2-dichloroethane.

TABLE 5.1.1.7.2

Reported vapor pressures of 1,2-dichloroethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)

$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)

$\log P = A - B/(C + T/K)$ (3)

$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Pearce & Peters 1929		**Stull 1947**		**Gutsche & Knapp 1982**	
isoteniscope method		**summary of literature data**		**Bourdon-tube manometer**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
–30.82	427	–44.5	133.3	28.75	12530
–24.92	613	–24.0	666.6	38.65	19521
–19.32	860	–13.6	1333	46.39	27004
–15.02	1093	–2.40	2666	51.72	33373
–10.42	1547	10.0	5333	56.63	40285
–5.12	2120	18.1	7999	60.79	47009
0.070	2800	29.4	13332	64.19	53158
5.09	3760	45.7	26664	67.62	60006
10.07	4893	64.0	53329	70.24	65669
15.52	6546	82.4	101325	73.85	74207
20.21	8279			76.36	80633
25.25	10639	mp/°C	–35.3	78.67	86926
30.23	13452			80.80	93115
35.24	16839			82.74	98997
39.79	20425			84.54	104743
45.13	25544				
51.12	31304			eq. 3	P/kPa
55.22	37997			A	14.142372
60.28	45969			B	2896.480
65.27	55035			C	52.506
70.27	65448				
75.36	77220				
80.43	91046				
85.45	105938				
91.03	124603				
bp/°C	84.1				
$\Delta H_V/(kJ\ mol^{-1}) = 32.41$ at bp					
vapor pressure eq. see ref.					

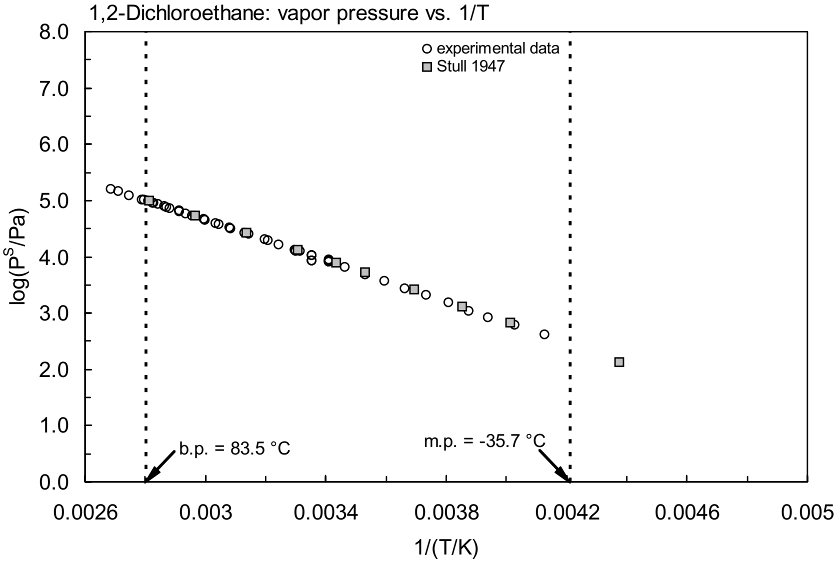


FIGURE 5.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichloroethane.

TABLE 5.1.1.7.3
Reported Henry's law constants of 1,2-dichlorethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)
$\ln H = A - B/(T/K)$ (4) $\log H = A - B/(T/K)$ (4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

Leighton & Calo 1981		Ashworth et al. 1988		Dewulf et al. 1995	
equilibrium cell-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.0	55.85	10	118.6	2.0	32.03
1.3	56.34	15	131.7	6.0	42.47
11.0	84.92	20	148.95	10.0	39.55
21.0	125.6	25	142.87	18.2	75.4
22.0	139.7	30	176.3	25.0	102.1
27.2	174.1				
25	119.3	eq. 4	H/(atm m³/mol)	eq. 1	K_{AW}
		A	−1.371	A	11.377
eq. 3	H/atm	B	1522	B	4329
A	16.05				
B	3539				

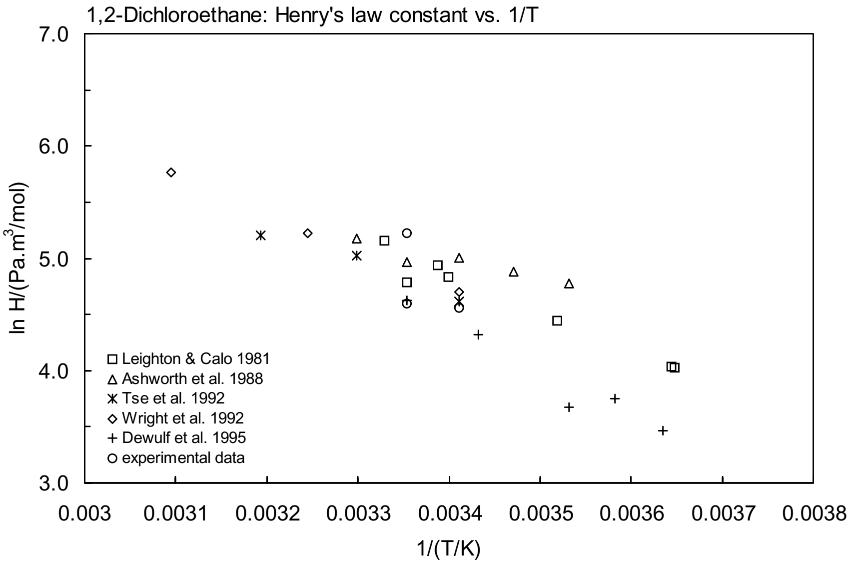


FIGURE 5.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dichloroethane.

TABLE 5.1.1.7.4
Reported octanol-water partition coefficients of 1,2-dichloroethane at various temperatures

Bhatia & Sandler 1995		DeWulf et al. 1999	
relative GC-RT technique		EPICS-GC	
t/°C	log K_{OW}	t/°C	log K_{OW}
25	1.51	2.2	1.43
35	1.51	4.0	1.46
50	1.53	10.0	1.47
		14.1	1.44
		18.7	1.50
		24.8	1.46
		change in enthalpy: $\Delta H_{OW}/(kJ\ mol^{-1})$ = 3.3 (–2.1 to 8.6) enthalpy of transfer $\Delta H_{oct}/(kJ\ mol^{-1})$ = 0.2. (–5.2 to 5.5)	

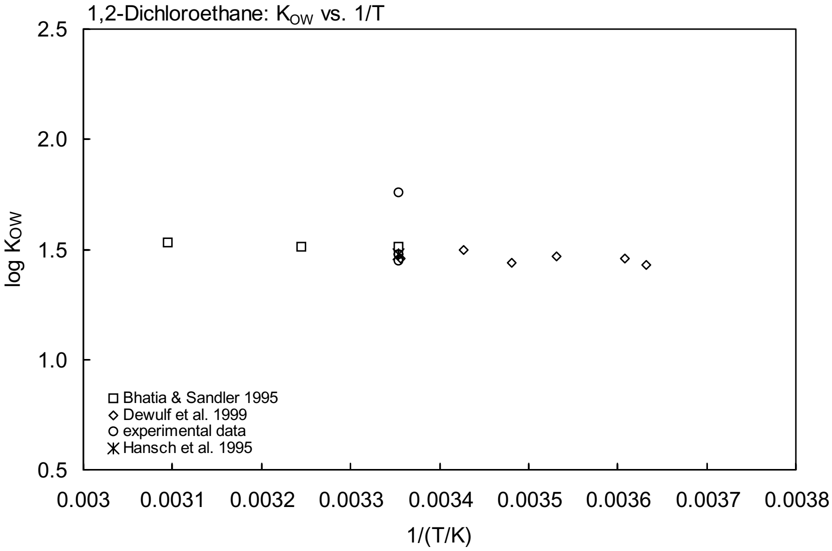
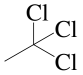


FIGURE 5.1.1.7.4 Logarithm of K_{OW} versus reciprocal temperature for 1,2-dichloroethane.

5.1.1.8 1,1,1-Trichloroethane



Common Name: 1,1,1-Trichloroethane
Synonym: methyl chloroform, chlorotene, Genklene, Baltana
Chemical Name: 1,1,1-trichloroethane
CAS Registry No: 71-55-6
Molecular Formula: CH_3CCl_3
Molecular Weight: 133.404
Melting Point (°C):
–30.01 (Lide 2003)
Boiling Point (°C):
74.09 (Lide 2003)
Density (g/cm^3 at 20°C):
1.3390 (Dreisbach 1961; Horvath 1982; Weast 1982–83; McNally & Grob 1984)
1.3381, 1.3299 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
99.0, 52.0 (calculated-density, intrinsic volume-van der Waals method, Abernethy et al. 1988)
100.0 (calculated-density, Wang et al. 1992)
114.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
32.74, 29.74 (25°C, bp, Dreisbach 1961)
32.39, 29.708 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
2.35 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1320* (20°C, shake flask, measured range 0–50°C, Van Arkel & Vles 1936)
1304 (Seidell 1940)
1490* (shake flask-GC, measured range 10–80°C, Walraevens et al. 1974)
log [S/(mol/L)] = 2070/(T/K) – 14.860 + 0.020·(T/K); temp range 2630353 K (shake flask, Walraevens et al. 1974)
480 (20°C, shake flask-GC, Pearson & McConnell 1975; McConnell et al. 1975)
880, 720 (1.5, 25°C, average literature values, Dilling 1977)
1360 (shake flask, Chiou et al. 1979)
1320 (20°C, recommended, Sørensen & Arit 1979)
100 (shake flask-titration, Coca & Diaz 1980)
1334 (shake flask-LSC, Banerjee et al. 1980)
1150, 1200 (23.5°C, elution chromatography, Schwarz 1980)
1850* (20°C, elution chromatography, measured range 10–30°C, Schwarz & Miller 1980)
1334; 278.7 (shake flask-LSC; calculated-f const., Veith et al. 1980)
1260 (calculated-group contribution as per Irmann 1965, Horvath 1982)
1485* (summary of literature data, temp range 0–80°C, Horvath 1982)
3200 (calculated-UNIFAC activity coeff., Arbuckle 1983)
479.8 (30°C, headspace-GC, McNally & Grob 1984)
1334 (calculated-UNIFAC activity coeff., Banerjee 1985)
1320 (20°C, selected, Riddick et al. 1986)
1310, 1194, 1267 (20, 35, 50°C, infinite dilution activity coeff. γ^{∞}-GC, Barr & Newsham 1987)
1252 (23–24°C, shake flask-GC, Broholm et al. 1992)
700* (20.2° C, shake flask-GC/TC, measured range 0–71.5°C, Stephenson 1992)

1260, 1353, 1370 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
1413, 1392, 1454, 1489 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
2935, 3228, 3536, 3749 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
1758 (γ^∞ from gas stripping-GC, Li et al. 1993)
1250 (shake flask-GC, Broholm & Feenstra 1995)
1380 (20°C, activity coeff. γ^∞ by inert air stripping-GC, Hovorka & Dohnal 1997)
1290* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = $1.09092 - 6.52776 \times 10^{-3}\cdot(T/K) + 1.10747 \times 10^{-5}\cdot(T/K)^2$, temp range 273–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are complied at the end of this section):
12159* (17.68°C, static method-Hg manometer, measured range 268–290 K, Rubin et al. 1944)
log (P/cmHg) = 6.92013 – 1729/(T/K); temp range 268–290 K (Hg manometer, Rubin et al. 1944)
16190* (interpolated from Antoine eq. regression, temp range –52 to 74.1°C, Stull 1947)
16100 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.94983 – 1217.0/(225.0 + t/°C); temp range –3 to 111°C (Antoine eq. for liquid state, Dreisbach 1961)
16170 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 8012.7/(T/K)] + 7.955902; temp range –52 to 74.1°C (Antoine eq., Weast 1972–73)
16490* (ebulliometry, measured range –77.15 to 25°C, Ambrose et al. 1975)
16490 (ebulliometry, measured –77.15 to 25°C, Boublik et al. 1984)
17800 (calculated-Antoine eq., Boublik et al. 1973, 1984)
log (P/mmHg) = 8.64344 – 2136.621/(302.769 + t/°C); temp range –5.36 to 16.92°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
12800 (20°C, Pearson & McConnell 1975; McConnell et al. 1975)
17800, 16490 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.78612 – 2147.034/(303.568 + t/°C); temp range –5.36 to 16.92°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.13297 – 1260.034/(231.327 + t/°C); temp range –77.2 to 25°C (Antoine eq. from reported exptl. data of Ambrose et al. 1973, Boublik et al. 1984)
log (P/mmHg) = 8.6434 – 2136.6/(302.8 + t/°C); temp range –6 to 17°C (Antoine eq., Dean 1985, 1992)
16490 (selected, Riddick et al. 1986)
log (P/kPa) = 5.98755 – 1182.527(222.594 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
16490 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.98755 – 1182.527/(–50.256 + T/K); temp range; 295–372 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.00452 – 1193.604/(–48.734 + T/K); temp range 349–408 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.36873 – 1474.394/(–8.08 + T/K); temp range 399–487 K (Antoine eq.-III, Stephenson & Malanowski 1987)
16530, 960 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
13150, 20520, 25300, 30940 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = $36.5468 - 2.821 \times 10^3/(T/K) - 10.205\cdot\log(T/K) - 2.6369 \times 10^{-9}\cdot(T/K) + 3.7075 \times 10^{-6}\cdot(T/K)^2$; temp range 243–545 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1638 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
3433 (20°C, McConnell et al. 1975)
2800, 2875 (exptl., calculated-P/C, Dilling 1977)
2025 (20°C, batch stripping-GC, Mackay et al. 1979)
730 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
log (k_H/atm) = 9.39 – 1992.95/(T/K), (least-square regression of data from lit., Kavanaugh & Trussell 1980)
1996* (equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)

ln (k_H/atm) = 21.68 – 4375/(T/K); temp range 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
1520 (20°C, batch air stripping, Munz & Roberts 1982)
836, 1317, 2155 (10, 20, 30°C, multiple equilibrium-GC, Munz 1985)
606.9 (20°C, predicted-UNIFAC activity coeff., Arbuckle 1983)
1319* (multiple equilibrium technique-GC, temp range 5–33°C, Hunter-Smith et al. 1983)
ln K_{AW} = 9.15 – 2915/(T/K); measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)
ln K_{AW} = 13.04 – 3905/(T/K); measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith 1983)
1743 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
1337, 1358 (20°C, EPICS-GC/FID, batch air stripping-GC, Lincoff & Gossett 1984)
ln [H/(atm m^3/mol)] = 10.21 – 4262/(T/K); temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)
ln [H/(atm m^3/mol)] = 9.975 – 4186/(T/K); temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)
498.5 (adsorption isotherm, Urano & Murata 1985)
1360 (20°C, multiple equilibration, Munz & Roberts 1986; quoted, Yurteri et al. 1987)
log K_{AW} = 5.327 – 1636/(T/K); temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)
498.5 (gas stripping-GC, Warner et al. 1987)
1345, 1413* (20, 25°C, EPICS-GC/FID, measured range 9.6–24.6°C, Gossett 1987)
ln [H/(atm m^3/mol)] = 9.777 – 4133/(T/K); temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)
1572 (20°C, EPICS, Yurteri et al. 1987)
1763* (EPICS-GC, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 7.351 – 3399/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
1317 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
1578* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
ln (1/K_{AW}) = –2.52 + 950/(T/K); temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
1277, 2027, 2381, 2847 (20, 30, 35, 40°C, from measured activity coeff. γ^∞-GC, Tse et al. 1992)
1380, 1998, 2952 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
1763* (26.3°C, EPICS-GC, measured range 26.3–44.8°C, Hansen et al. 1993)
ln [H/(kPa·m^3/mol)] = –3120/(T/K) + 11.0; temp range 26.3–45°C (EPICS-GC, Hansen et al. 1993)
1783* (static headspace-GC, measured range 25–50°C, Robbins et al. 1993)
1507* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)
800, 2010 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
ln K_{AW} = –3834/(T/K) + 0.00897·Z + 12.351; with Z salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID measurements, Dewulf et al. 1995)
1387 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
2072 (vapor-liquid equilibrium-GC, Turner et al. 1996)
K_{AW} = 0.204 + 0.0182·(T/K) + 0.000173·(T/K)^2; temp range 0–35°C (vapor-liquid equilibrium-GC with additional lit. data, Turner et al. 1996)
1280 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)
1614, 1750, 1415; 1380 (direct calculated method, gas-phase EPICS method, liquid-phase EPICS method; quoted lit. Chiang et al. 1998)
1370 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 5.163 – 1588/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.17 (Tute 1971)
2.49 (shake flask, Hansch & Leo 1979; Hansch & Leo 1985)
2.47 (shake flask-LSC, Banerjee et al. 1980)
2.47 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982)
2.35, 2.29 (calculated-UNIFAC with octanol and water mutual solubility not considered, calculated-UNIFAC with octanol and water mutual solubility considered, Arbuckle 1983)
1.96 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
2.49 (recommended, Sangster 1993)
2.60 (calculated-activity coefficients, Tse & Sandler 1994)

2.47* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
2.20* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
2.70 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
1.40 (calculated-K_{OW}, Veith et al. 1979; Veith et al. 1980)
0.954 (bluegill sunfish, Veith et al. 1980)
0.954 (bluegill sunfish, Barrows et al. 1980)
1.908 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
0.950 (bluegill sunfish, Veith & Kosian 1982)
1.70 (calculated-MCI χ, Koch 1983)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
2.02 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
2.25 (quoted from Chiou et al. 1979, Karickhoff 1981,1985)
2.08, 2.04, 2.02 (estimated-K_{OW}, estimated-S and mp, estimated-S, Karickhoff 1981)
2.182 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
2.20 (soil, best estimate, Karickhoff 1985)
1.70 (calculated-MCI χ, Bahnick & Doucette 1988)
2.26 (20°C, soil, Chiou et al. 1988)
1.65 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
2.22 (20°C, weathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
3.02 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
2.053 (soil, selected, Jury et al. 1990)
1.95, 1.98, 1.98, 1.99, 2.01, 1.98, 2.03 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon f_{OC} = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)
3.20 (soil, calculated-universal solvation model, Winget et al. 2000)
2.16 (soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Sorption Partition Coefficient, logK_{OM}:
2.02, 1.55 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2}$(exptl) = 21 min, $t_{1/2}$(calc) = 0.34 min from water (Dilling et al. 1975)
$t_{1/2}$(exptl) ~ (20 ± 3) min at 25°C for an aqueous solution of 1 mg L^{-1} when stirred at 200 rpm in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);
Evaporation $t_{1/2}$(exptl) = (17.3–24.9) min, $t_{1/2}$(calc) = 0.19 min, 23.7 min at 20–25°C, and $t_{1/2}$ = 30.2 min at 15°C from water (Dilling 1977);
estimated $t_{1/2}$ ~ 3.7 h from water (Thomas 1982);
k = 0.029 d^{-1}, $t_{1/2}$ = 24 d in spring at 8–16°C, k = 0.058 d^{-1}, $t_{1/2}$ = 12 d in summer at 20–22°C, k = 0.063 d^{-1}, $t_{1/2}$ = 11 d in winter at 3–7°C for the periods when volatilization appears to dominate, and k = 0.60 d^{-1}, $t_{1/2}$ = 11.5 d with $HgCl_2$, and k = 0.072 d^{-1}, $t_{1/2}$ = 9.6 d without $HgCl_2$ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);
estimated $t_{1/2}$ ~ 365 d for volatilization loss from soil to be 365 d (Jury et al. 1990).

Photolysis: not expected to be important (Howard et al. 1991).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$k_{OH} = 3.36 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} with a troposphere life time of 1.1 yr at 298 K (relative rate method, Cox et al. 1976; quoted, Callahan et al. 1979)
$k_{OH} = (1.5 \pm 0.3) \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow-resonance fluorescence, Howard & Evenson 1976b)

k_{OH}* = (2.19 ± 0.26) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 275–405 K, with calculated lifetime of 3.8–6.0 yr in troposphere (discharge flow system-resonance fluorescence, Chang & Kaufman 1977)

k_{OH} = (1.59 ± 0.16) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 298 K with lifetime of 13 yr (flash photolysis-resonance fluorescence, Watson et al. 1977; quoted, Callahan et al. 1979; Altshuller 1980)

k_{OH}* = (1.06 ± 0.09) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 293 K, measured range 278–461 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1979)

k_{OH}* = (1.08 ± 0.20) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 222–363 K (flash photolysis resonance fluorescence, Kurylo et al. 1979)

k_{OH} = 1.0 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1}, with an estimated toxic chemical residence time of 1160 d, loss < 0.1% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et at. 1981)

k = 9.0 × 10^9 cm^3 mol^{-1} s^{-1}, estimated at 300 K (Lyman 1982)

k << 360 M^{-1} h^{-1} for singlet oxygen and 1.0 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation $t_{½}$ = 5393–53929 h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

k_{OH}(calc) = 1.3 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.19 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1987)

k_{OH}* = 1.19 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH} = 1.19 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} with a troposphere lifetime of 1.7 yr for a global average concentration of OH radical (Prinn et al. 1987; quoted, Bunce et al. 1991)

k_{O3}(aq.) ≤ 0.012 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{½}$ ≥ 32 d at pH 7 (Yao & Haag 1991).

Hydrolysis: k = 0.12 $month^{-1}$ with $t_{½}$(exptl.) = 6 months at pH 7 and 25°C (Dilling et al. 1975; quoted, Callahan et al. 1979; Mabey et al. 1979; Neely 1985);

k = 0.96 yr^{-1} at pH 7 and 25°C with a first-order hydrolysis $t_{½}$ = 0.73 yr (Kollig et al. 1987);

k = (1.93 ± 0.40) × 10^{-8} s^{-1} in distilled water contained 0.1% w/w CH_2O as sterilant with 39% conversion, k = (2.04 ± 0.47) × 10^{-8} s^{-1} in autoclaved distilled water with 40% conversion and k = (1.80 ± 0.90) × 10^{-8} s^{-1} in sediment contained 0.1% w/w CH_2O as sterilant with 25% conversion at 25°C, calculated $t_{½}$ = 350 d at 25°C (Haag & Mill 1988)

$t_{½}$ = 6 months, abiotic hydrolysis or dehydrohalogenation half-life (Olsen & Davis 1990)

$t_{½}$ = 0.73 yr, based on reported rate constant at pH 7 at 25°C(Howard et al. 1991)

Biodegradation:

k = 0.043 d^{-1} in fresh water plus sediment incubated under anaerobic conditions (Wood et al. 1981; quoted, Klečka 1985);

$t_{½}$(aq. aerobic) = 3360–6552 h, based on unacclimated aerobic seawater grab sample data and sub-soil sample data from a ground water aquifer (Pearson & McConnell 1975; Wilson et al. 1983; quoted, Howard et al. 1991);

$t_{½}$(aq. anaerobic) = 13440–26208 h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{½}$ = 26 wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

estimated troposphere residence time of 1.1 yr for reaction with OH radical (CEQ 1975);

estimated N. troposphere residence time of 7.2 yr by one compartment non-steady state model (Singh et al. 1978);

estimated troposphere residence time of 8–10 yr by two compartment non-steady state model (Singh 1977; Singh et al. 1979);

lifetime of 8 yr in troposphere (Altshuller 1980);

estimated toxic chemical residence time of 1160 d, loss < 0.1% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et at. 1981)

atmospheric lifetime τ = 6.3 yr (Prinn et al. 1987);

troposphere lifetime of 1.7 yr for a global average concentration of OH radical (Bunce et al. 1991)

$t_{½}$ = 5393–53929 h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

estimated tropospheric lifetime of 7.8 yr and 6.1 yr by rigorous calculations (Nimitz & Skaggs 1992).

Surface water: $t_{½}$ = 24 d in the spring at 8–16°C, $t_{½}$ = 12 d in the summer at 20–22°C, $t_{½}$ = 11 d in the winter at 3–7°C when volatilization dominates, and $t_{½}$ = 11.5 d and 9.6 d for experiments with and without $HgCl_2$ as poison, respectively, in September 9–15 in marine mesocosm experiment (Wakeham et al. 1983);

calculated hydrolysis $t_{½}$ = 350 d at 25°C (Haag & Mill 1988);

$t_{½}$ = 3360–6552 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

k(exptl) ≤ 0.012 $M^{-1}\,s^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{½} \geq 32$ d at pH 7 (Yao & Haag 1991).

Ground water: estimated $t_{½}$ ~ 1.0 yr in the groundwater of the Netherlands (Zoeteman et al. 1981);

$t_{½}$ = 3360–13104 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and sub-soil grab sample data from a ground water aquifer (Howard et al. 1991; Wilson et al. 1983).

Sediment: measured $t_{½}$ = 450 d at 25°C, based on neutral and base-catalyzed hydrolysis rates studied in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil: $t_{½}$ = 365 d, estimated volatilization loss (Jury et al. 1990);

$t_{½}$ = 3360–6552 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{½}$ < 1 d in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 5.1.1.8.1
Reported aqueous solubilities of 1,1,1-trichloroethane at various temperatures

$$S/(wt\%) = 0.1910 - 2.2811 \times 10^{-3}\cdot(t/°C) + 2.5529 \times 10^{-5}\cdot(t/°C)^2 - 2.4775 \times 10^{-8}\cdot(t/°C)^3 \quad (1)$$

$$S/(wt\%) = 1.09092 - 6.52776 \times 10^{-3}\cdot(T/K) + 1.10747 \times 10^{-5}\cdot(T/K)^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Schwarz & Miller 1980		Horvath 1982	
shake flask		shake flask-GC		elution chromatography		summary of literature data	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
0	1590	10	1730	10	1800	0	1910
20	1320	20	1550	20	1850	10	1707
35	1260	25	1490	30	1590	20	1554
50	1280	30	1440			25	1495
		40	1390			30	1449
		50	1380			40	1390
		60	1410			50	1377
		70	1480			60	1407
		80	1590			70	1479
						80	1592
						eq. 1	S/wt%

TABLE 5.1.1.8.1 (*Continued*)

2.

Barr & Newsham 1987		Stephenson 1992		Tse et al 1992		Horvath & Getzen 1999a	
activity coefficient		shake flask-GC		activity coefficient		recommended, IUPAC-NIST	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	1310	0	1470	20	1413	0	1340
35	1194	20.2	700	30	1392	5	1320
50	1267	31.6	760	35	1454	10	1300
		41.1	1010	40	1489	15	1290
		51.3	1060			20	1290
		61.5	1030			25	1290
		71.5	1140	**Wright et al. 1992**		30	1300
				activity coefficient		35	1310
				t/°C	**S/g·m^{-3}**	40	1330
						45	1350
				20	1260	50	1380
				30	1353		
				40	1370	eq. 2	S/wt%
						temp range 273–323 K	

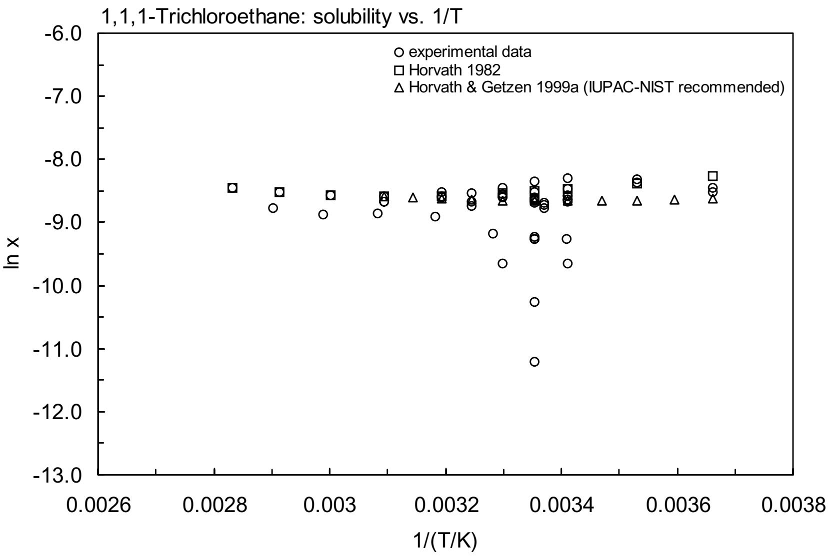


FIGURE 5.1.1.8.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.2
Reported vapor pressures of 1,1,1-trichloroethane at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		

Rubin et al. 1944		Stull 1947		Ambrose et al. 1975	
static-mercury manometer		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–5.534	3840	–52.0	133.3	–77.15	20
–0.207	5160	–32.0	666.6	–55.15	100
5.12	6733	–21.9	1333	–25.85	1000
11.33	9239	–10.8	2666	14.15	10000
16.93	12159	1.6	5333	25.0	16490
		9.5	7999		
mp/K	240.2	20.0	13332		
		36.2	26664		
eq. 1	P/cmHg	54.6	53329		
A	6.92013	74.1	101325		
B	1729				
		mp/°C	–30.6		
$\Delta H_V/(kJ\ mol^{-1})$ = 33.42					
at 286.53 K					

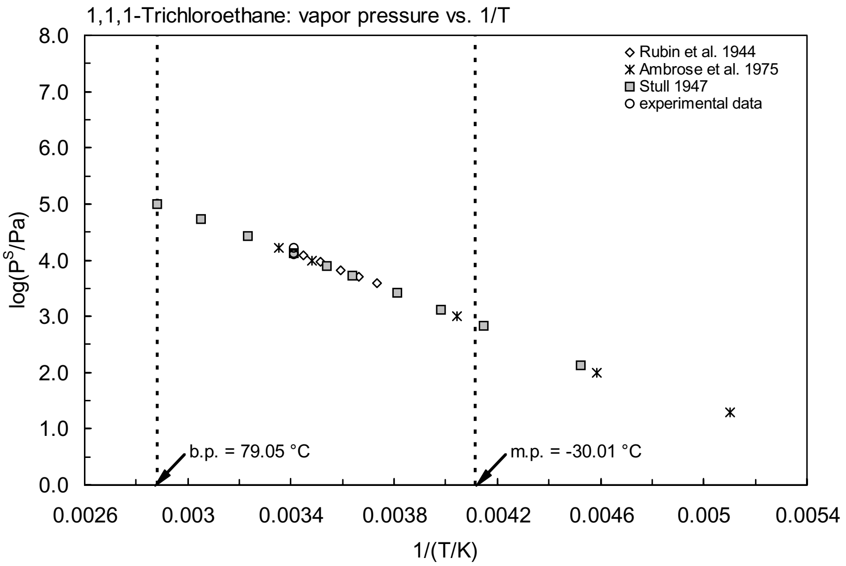


FIGURE 5.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.3
Reported Henry's law constants of 1,1,1-trichloroethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)
$\ln H = A - B/(T/K)$ (4) $\log H = A - B/(T/K)$ (4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

1.

Leighton & Calo 1981		Hunter-Smith 1983		Gossett 1987		Ashworth et al. 1988	
equilibrium cell-GC		multiple equilibrium-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
1.0	541.7	5	612	9.6	771	10	978
1.0	543.3	10	749	17.5	1216	15	1165
1.2	555.9	15	912	24.8	1743	20	1479
2.5	597.9	20	1102	34.6	2523	25	1763
7.0	763.3	25	1324			30	2138
10.0	919.2	33	1738	eq. 4	H/(atm m^3/mol)		
12.0	1016			A	9.777	eq. 4	H/(atm m^3/mol)
12.0	1039			B	4133	A	7.351
12.9	1069					B	3399
14.0	1190						
18.0	1398						
18.0	1447						
18.0	1464						
19.0	1511						
19.2	1526						
19.5	1437						
24.3	1874						
25.2	1995						
25.3	2026						
26.0	1988						
26.0	2064						
26.1	1958						
$\ln (k_H/\text{atm}) = A - B/(T/K)$							
A	21.68						
B	4375						

2.

Kolb et al. 1992		Tse et al. 1992		Wright et al. 1992		Hansen et al. 1993	
equilibrium headspace-GC		activity coefficient		activity coefficient		EPICS-GC	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
40	1578	20	1277	20	1380	26.3	1763
60	1884	30	2027	30	1998	35.0	2412
70	2264	35	2381	40	2952	44.8	3232
80	2488	40	2847				
						eq. 4	H/(kPa m^3/mol)
eq. 2	1/K$_{AW}$					A	11 ± 0.30
A	–2.52					B	3120 ± 93
B	–950						

(*Continued*)

TABLE 5.1.1.8.3 (*Continued*)

3.

Robbins et al. 1993		Dewulf et al. 1995	
static headspace-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
25	1783	2.0	152.1
30	2209	6.0	195.2
40	2675	10.0	194.7
45	3597	18.2	378.2
50	4164	25.0	510.6
		eq. 1	K_{AW}
		A	12.351
		B	3834

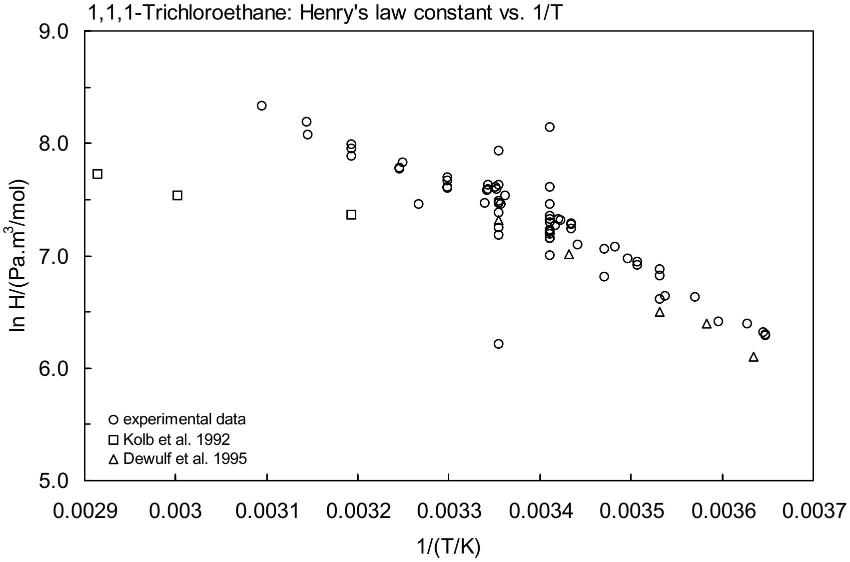


FIGURE 5.1.1.8.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.4
Reported octanol-water partition coefficients of 1,1,1-trichloroethane at various temperatures

Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		shake flask-GC	
t/°C	log K_{OW}	t/°C	log K_{OW}
25	2.47	2.2	2.18
35	2.50	6.0	2.18
50	2.52	10.0	2.28
		14.1	2.24
enthalpy of transfer		18.7	2.285
$\Delta H/(kJ\ mol^{-1}) = -20.2$		24.8	2.20
log $K_{OW} = A - \Delta H/2.303RT$			
A	1.0195		
ΔH	–20.2		

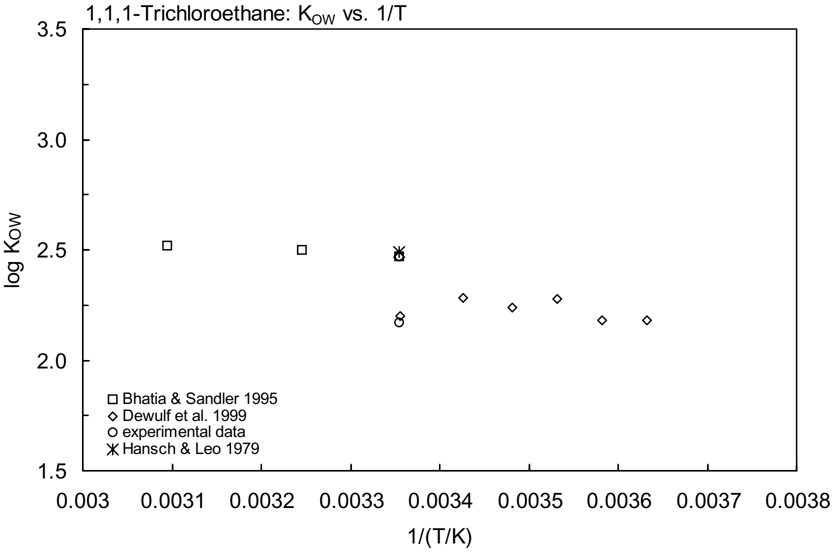
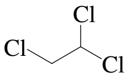


FIGURE 5.1.1.8.4 Logarithm of K_{OW} versus reciprocal temperature for 1,1,1-trichloroethane.

5.1.1.9 1,1,2-Trichloroethane



Common Name: 1,1,2-Trichloroethane
Synonym: vinyl trichloride
Chemical Name: 1,1,2-trichloroethane
CAS Registry No: 79-00-5
Molecular Formula: $CH_2ClCHCl_2$
Molecular Weight: 133.404
Melting Point (°C):
–36.3 (Lide 2003)
Boiling Point (°C):
113.8 (Lide 2003)
Density (g/cm^3 at 20°C):
1.440 (Dreisbach 1959; Weast 1982–83; Verschueren 1983;)
1.43931, 1.43213(20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
93.0 (calculated-density, Wang et al. 1992)
114.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
46.77, 37.07 (25°C, bp, Dreisbach 1961)
40.28, 34.23 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.543 (Dreisbach 1959; quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are complied at the end of this section):
3704 (volumetric method, Wright & Schaffer 1932)
4580* (shake flask, measured range 0–55°C, Van Arkel & Vles 1936)
4418 (Seidell 1940)
4400 (data presented in graph, temp range 0–70°C, McGovern 1943)
4400 (shake flask-refractive index and density, Treybal et al. 1946)
4380* (shake flask-GC, measured range 0–80°C, Walraevens et al. 1974)
$\log [S/(mol/L)] = 2070/(T/K) - 15.285 + 0.0230 \cdot (T/K)$; temp range 0–80°C (Walraevens et al. 1974)
4420 (literature average, Dilling 1977)
4500 (20°C, Verschueren 1977, 1983)
4370 (20°C, recommended, Sørensen & Arit 1979)
5100 (shake flask-titration/turbidity, Coca & Diaz 1980, Coca et al. 1980)
1490 (shake flask-LSC, Veith et al. 1980)
4394* (summary of literature data, temp range 0–80°C, Horvath 1982)
4365 (30°C, headspace-GC, McNally & Grob 1984)
4800 (Dean 1985)
4941, 4876, 5183 (20, 35, 50°C, infinite dilution activity coeff. γ^∞-GC, Barr & Newsham 1987)
2858, 1469 (predicted-MCI χ and polarizability, Nirmalakhandan & Speece 1988)
4580* (31.3°C, shake flask-GC/TC, measured range 0–90.8°C, Stephenson 1992)
4813, 5035, 5205 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
2574, 2960, 3378 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
4877, 5257, 6075 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
4460 (20°C, activity coeff. γ^∞ by inert air stripping-GC, Hovorka & Dohnal 1997)

4590* (tentative values, temp range 0–55°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = $2.89796 - 1.8585 \times 10^{-2}\cdot(T/K) + 3.48961 \times 10^{-5}\cdot(T/K)^2$, temp range 273–328 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):
26664* (73.5°C, ebulliometry, measured range 73.5–113.5°C, Treybal et al. 1946)
3090* (Antoine eq. regression, temp range –24 to 113.9°C, Stull 1947)
19114* (49.97°C, ebulliometry, measured range 49.97–113.67°C, Dreisbach & Shrader 1949)
2998 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.84165 – 1262.6/(205.0 + t/°C); temp range 30–186°C (Antoine eq. for liquid state, Dreisbach 1959)
3217 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.96527 – 1351.0/(217.0 + t/°C); temp range 29–155°C (Antoine eq. for liquid state, Dreisbach 1961)
3088 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9163.2/(T/K)] + 8.079996; temp range –24 to 113.9°C, (Antoine eq., Weast 1972–73)
2910 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
log (P/mmHg) = 6.95185 – 1314.41/(209.197 + t/°C); temp range 49.97–113.7°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
3066 (literature average, Dilling 1977)
2533, 4266 (20, 30°C, Verschueren 1983)
log (P/kPa) = 6.13975 – 1313.598/(209.106 + t/°C); temp range 49.97–113.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
log (P/mmHg) = 6.95185 – 1314.41/(209.20 + t/°C); temp range 50–114°C (Antoine eq., Dean 1985, 1992)
2998 (selected lit., Riddick et al. 1986)
log (P/kPa) = 6.10301 – 1332.6/(211.38 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
3218 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.09017 – 1351.0/(–56.15 + T/K); temp range 302–428 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.13875 – 1351.685/(–59.953 + T/K); temp range 316–384 K (Antoine eq., Stephenson & Malanowski 1987)
2369, 4012, 6590 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = $25.0845 - 2.7368 \times 10^3/(T/K) - 5.9182\cdot\log(T/K) + 2.5155 \times 10^{-10}\cdot(T/K) + 1.1831 \times 10^{-6}\cdot(T/K)^2$; temp range 237–602 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
92.1 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
94.2 (calculated-P/C, Dilling 1977)
78.4 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
122, 120 (calculated-P/C, recommended, Mackay & Shiu 1981, 1990)
81.4* (24.3°C, equilibrium cell-concn ratio-GC/FID, measured range 2.5–26.1°C, Leighton & Calo 1981)
ln (k_H/atm) = 16.20 – 3690/(T/K); temp range 2.5–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
92.2* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 9.320 – 4943/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
74.97 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
97.34 (computed value, Yaws et al. 1991)
70.9, 115.5, 172.3 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
67.1, 136, 234 (20, 35, 50°C, activity coeff γ^∞-differential pressure transducer, Wright et al. 1992)
82* (26.2°C, EPICS-GC, measured range 26.2–44.8°C, Hansen et al. 1993)
ln [H/(kPa·m^3/mol)] = –5091/(T/K) + 17.0; temp range 26.2–45°C (EPICS-GC measurements, Hansen et al. 1993)

1.30, 2.48 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
122 (quoted from Howard 1989–1991, Capel & Larson 1995)
66.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1998)
65.7 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
66.78 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 5.219 - 1989/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperature designated * are compiled at the end of this section:
2.17 (calculated as per Tute 1971, Callahan et al. 1979; Ryan et al. 1988)
2.38 (Hansch & Leo 1979)
1.89 (shake flask, Log P Database, Hansch & Leo 1987)
1.89 (recommended, Sangster 1993)
2.07 (calculated-activity coefficients, Tse & Sandler 1994)
1.98* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
1.89 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
3.40 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
< 1.0 (Kawasaki 1980; quoted, Howard 1990)
1.519 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
1.23 (quoted, Isnard & Lambert 1988)
1.049 (calculated-K_{OW}, McCarty et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
1.845 (sandy soil column, Wilson et al. 1981)
1.748 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
3.20; 1.90 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
1.88 (soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2}$ = 21 min, estimated from lab. experiment of initial 1 mg/L in water stirred at 200 rpm at 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982; Howard 1990)
Evaporation $t_{1/2}$(exptl) = 35.1 min, $t_{1/2}$(calc) = 6.1 min, 30.1 min from water (Dilling 1977)
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k_{OH}* = $(3.18 \pm 0.06) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 295 K, measured range 278–461 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1979)
$k_{OH} = 3.3 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, with estimated residence time of 35 d, loss of 2.8% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
k << 360 M^{-1} h^{-1} for singlet oxygen and k = 3.0 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)
photooxidation $t_{1/2}$ ~ 196–1956 h, based on measured rate constants for reaction with hydroxyl radical in air (estimated, Atkinson 1985; quoted, Howard et al. 1991)
k_{OH}* = $(3.18 \pm 0.2) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 295 K, measured range 277–461 K (discharge flow-resonance fluorescence, Jeong et al. 1984)
k_{O3}(aq.) ≤ 0.08 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2}$ ≥ 5 d at pH 7 (Yao & Haag 1991).
k_{OH}(aq.) = 1.1×10^8 M^{-1} h^{-1} for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

Hydrolysis:

$k = 1.2 \times 10^{-7}$ h^{-1} at 25°C and pH 7 (estimated, Mabey et al. 1982)

$k = 5.9 \times 10^{-3}$ M^{-1} s^{-1} with $t_{1/2}$ = 3263 h, based on alkaline catalyzed hydrolysis reaction at pH 9 and 25°C; $t_{1/2}$ = 37 yr, based on hydrolysis rate constant measured at pH 7 and 25°C (Mabey et al. 1983; quoted, Howard 1990; Howard et al. 1991)

$t_{1/2}$(abiotic) or $t_{1/2}$(dehydrohalogenation) = 170 months (Olsen & Davis 1990)

$t_{1/2}$ = 14000 d at pH 7, $t_{1/2}$ = 0.14 d at pH12 in natural waters (Capel & Larson 1905)

Biodegradation:

$t_{1/2}$(aq. aerobic) = 4320–8760 h, based on the extremely low or no biodegradation which was observed in screening tests and a river die-away test (Tabak et al. 1981; Kawasaki 1980; Mudder & Musterman 1982; quoted, Howard 1990; Howard et al. 1991)

$t_{1/2}$(aq. anaerobic) = 17280–35040 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991)

$k = 0.04$ yr^{-1} with $t_{1/2}$ = 24 d (Wood et al. 1985; quoted, Olsen & Davis 1990)

$t_{1/2}$(aerobic) = 180 d, $t_{1/2}$(anaerobic) = 720 d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant $k = 3 \times 10^{-12}$ mL cell^{-1} h^{-1} for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 0.763$ h^{-1} (flagfish, calculated-BCF × k_2, McCarty et al. 1992)

$k_2 = 0.0676$ h^{-1} (flagfish, estimated from one compartment first-order kinetic, McCarty et al. 1992)

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h for the reaction with OH radical in air (Darnall et al. 1976);

photodecomposition $t_{1/2}$ = 15.9 h with NO under simulated atmospheric conditions (Dilling et al. 1976);

estimated residence time of 35 d, loss of 2.8% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2}$ = 196–1956 h, based on measured rate constants for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: estimated $t_{1/2}$ = 1.9 d in surface waters in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2}$ = 3263–8760 h, based on estimated hydrolysis half-life at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and estimated unacclimated aerobic aqueous degradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2}$(aerobic) = 100 d, $t_{1/2}$(anaerobic) = 400 d and hydrolysis $t_{1/2}$ = 14000 d at pH 7, $t_{1/2}$ = 0.14 d at pH 12 in natural waters (Capel & Larson 1995)

k(exptl) ≤ 0.08 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 5$ d at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2}$ = 3263–117520 h, based on estimated hydrolysis half-life pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and data from estimated unacclimated aerobic aqueous biodegradation half-life as well as a ground water die-away study in which no biodegradation was observed (Wilson et al. 1984; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 3263–8760 h, based on estimated hydrolysis half-life at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991) and a soil column test in which no biodegradation was observed (Wilson et al 1981; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.1.9.1
Reported aqueous solubilities of 1,1,2-trichloroethane at various temperatures

$$S/(\text{wt\%}) = 0.48137 - 2.9594 \times 10^{-3}\cdot(t/°C) + 4.3162 \times 10^{-5}\cdot(t/°C)^2 + 3.2190 \times 10^{-7}\cdot(t/°C)^3 \quad (1)$$

$$S/(\text{wt\%}) = 2.89796 - 1.8585 \times 10^{-2}\cdot(T/K) + 3.48961 \times 10^{-5}\cdot(T/K)^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982		Barr & Newsham 1987	
shake flask				summary of literature data		activity coefficient	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
0	4660	10	4600	0	4814	20	4941
20	4360	20	4410	10	4546	35	4876
25	4580	25	4380	20	4420	50	5183
55	5320	30	4390	25	4394		
		40	4530	30	4401		
		50	4830	40	4527		
		60	5290	50	4815		
		70	5950	60	5287		
		80	6860	70	6961		
				80	6857		
				eq. 1	S/wt%		

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999a	
shake flask-GC		activity coefficient		activity coefficient		tentative, IUPAC-NIST	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
0	4640	20	4813	20	4877	0	4250
9.2	4390	30	5035	35	5257	5	4280
31.3	4580	40	5205	50	6075	10	4330
41	4830					15	4400
50.6	5180					20	4490
60.5	4970					25	4590
710	5550					30	4710
81.7	6380					35	4850
90.8	7030					40	5000
						45	5170
						50	5360
						55	5570
						eq. 2	S/wt%
						temp range 263–328 K	

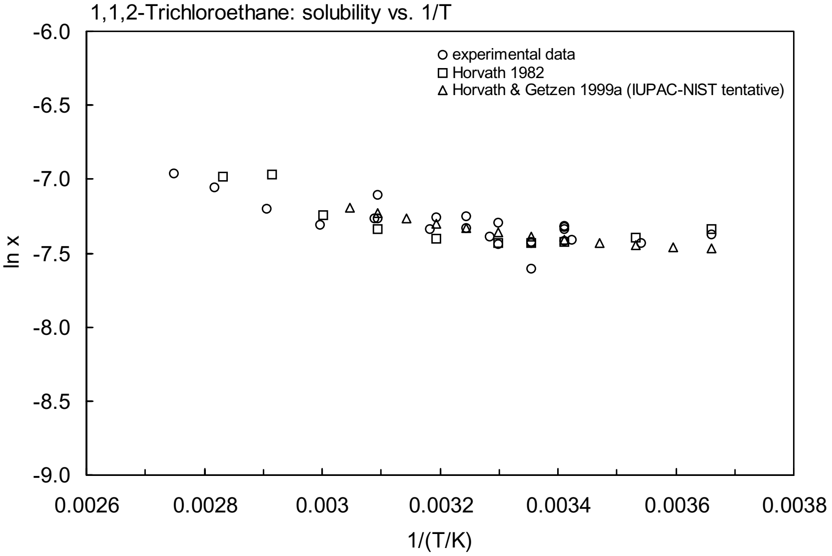


FIGURE 5.1.1.9.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.9.2
Reported vapor pressures of 1,1,2-trichloroethane at various temperatures

Treybal et al. 1946		Stull 1947		Dreisbach & Shrader 1949	
ebulliometry		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
73.5	26664	–24.0	133.3	49.97	19114
80.3	34397	–2.0	666.6	61.29	16500
82.4	37064	8.3	1333	85.99	42066
83.8	38530	21.6	2666	100.34	67661
85.6	41597	35.2	5333	113.67	101325
96.2	59328	44.0	7999		
104.6	77594	55.7	13332		
108.7	87326	73.3	26664		
109.8	90393	93.0	53329		
111.3	94392	113.9	101325		
113.5	101325				

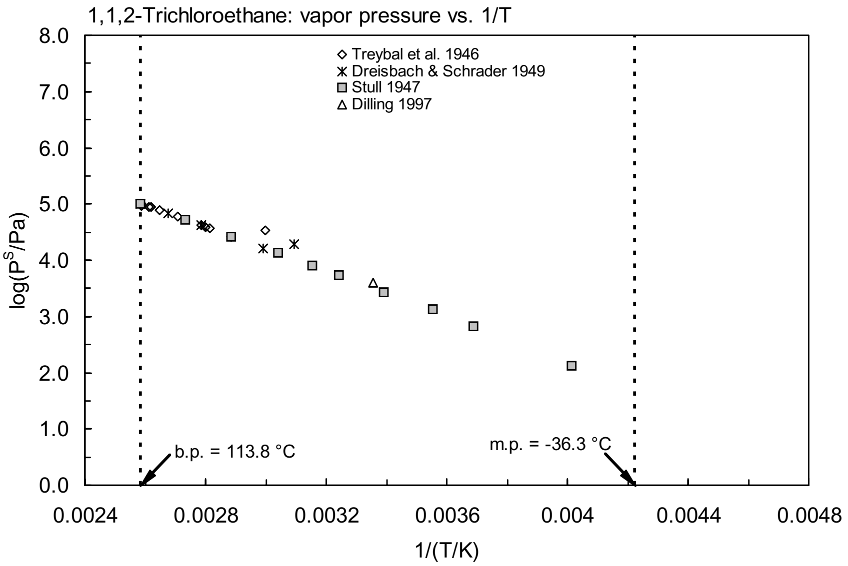


FIGURE 5.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.9.3
Reported Henry's law constants of 1,1,2-trichloroethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Leighton & Calo 1981		Ashworth et al. 1988		Tse et al. 1992		Hansen et al. 1993	
equilibrium cell-GC		EPICS-GC		activity coefficient		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
2.5	30.4	10	39.52	20	70.9	26.2	82
7.0	38.23	15	63.83	30	115.5	35.8	184
12.9	49.08	20	74.98	40	172.3	44.8	259
18.0	62.27	25	92.21				
19.5	61.35	30	134.76			eq. 4	H/(kPa m³/mol)
24.3	81.36			Wright et al. 1992		A	17 ± 3.36
26.1	88.4	eq. 4	H/(atm m³/mol)	activity coefficient		B	5901 ± 1158
		A	9.320	t/°C	H/(Pa m³/mol)		
eq. 3	k_H/atm	B	4843				
A	16.02			20	67.1		
B	3690			35	136		
				50	234		

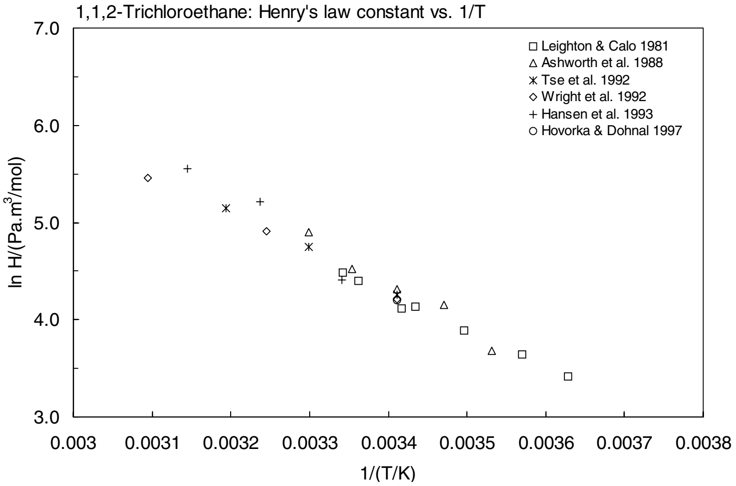


FIGURE 5.1.1.9.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.9.4
Reported octanol-water partition coefficients of 1,1,2-trichloroethane at various temperatures

	Bhatia & Sandler 1995
	relative GC-RT technique
t/°C	log K_{OW}
25	1.98
35	1.93
50	1.94

enthalpy of transfer

$\Delta H/(kJ\ mol^{-1}) = -20.2$.

$\log K_{OW} = A - \Delta H/2.303RT$

A	1.0195
ΔH	–20.2

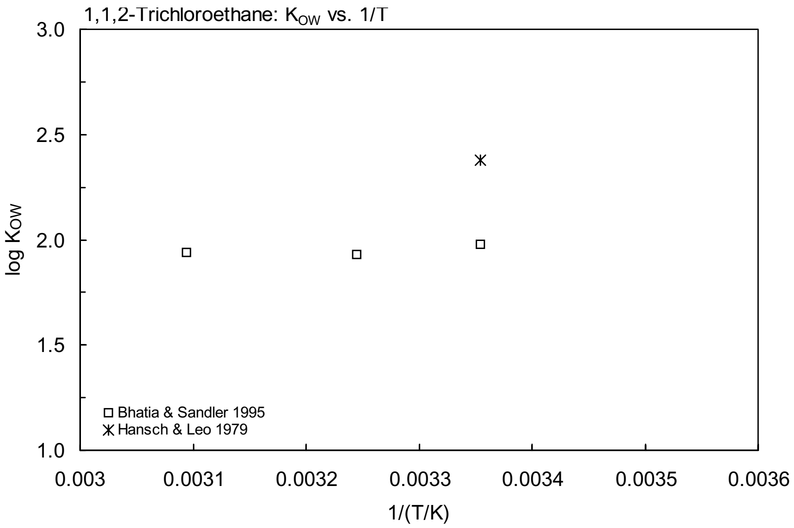
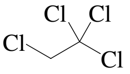


FIGURE 5.1.1.9.4 Logarithm of K_{OW} versus reciprocal temperature for 1,1,2-trichloroethane.

5.1.1.10 1,1,1,2-Tetrachloroethane



Common Name: 1,1,1,2-Tetrachloroethane
Synonym:
Chemical Name: 1,1,1,2-tetrachloroethane
CAS Registry No: 630-20-6
Molecular Formula: CH_2ClCCl_3
Molecular Weight: 167.849
Melting Point (°C):
–70.2 (Lide 2003)
Boiling Point (°C):
130.2 (Lide 2003)
Density (g/cm^3 at 20°C):
1.5406 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
1.5328 (25°C, Dreisbach 1961)
1.4819 (Dean 1985)
Molar Volume (cm^3/mol):
109.0 (20°C, calculated-density)
135.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
34.78, 42.18 (normal boiling point, 25°C, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are complied at the end of this section:
1090* (20°C, shake flask, measured range 0–50°C, Van Arkel & Vles 1936)
1110 (Seidell 1940)
1100* (shake flask, temp range 10–80°C, Walraevens et al. 1974)
log [S/(mol/L)] = 2070/(T/K) – 16.165 + 0.0236·(T/K), temp range 283–353 K (Walraevens et al. 1974)
1100 (interpolation of literature values, Dilling 1977)
215, 200, 202 (3, 20, 34°C, shake flask-GC, Chiou & Freed 1977)
1110* (summary of literature data, temp range 0–80°C, Horvath 1982)
1206, 1280, 1292, 1321 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
1178, 1382, 1492, 1607(20, 30, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
1005, 1093, 1056 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
1070* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 2.17896 – 1.3966 × 10^{-3}·(T/K) + 2.93282 × 10^{-5}·(T/K)^2, temp range 273–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1767* (Antoine eq. regression, temp range 58–200°C, Stull 1947)
8851* (59.31°C, ebulliometry, measured range 59.31–130.2°C, Dreisbach & Shrader 1949)
1578 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.97560 – 1410.7/(214.0 + t/°C); temp range 43–174°C (Antoine eq. for liquid state, Dreisbach 1961)
1778 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9296.5/(T/K)] + 7.938042; temp range –16.3 to 130.5°C (Antoine eq., Weast 1972–73)
1604 (calculated-Antoine eq., Boublik et al. 1973, 1984)

log (P/mmHg) = 6.89875 – 1365.876/(209.744 + t/°C); temp range 59–130°C (Antoine eq. from reported exptl. data of data of Dreisbach & Shrader 1949, Boublik et al. 1973)
1853 (20°C, interpolation of literature values, Dilling 1977)
log (P/kPa) = 6.02534 – 1366.919/(209.861 + t/°C); temp range 59.31–130.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
log (P/mmHg) = 6.89875 – 1365.88/(209.74 + t/°C); temp range 59–13 0°C(Antoine eq., Dean 1985, 1992)
1578 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.1005 – 1410.7/(–59.15 + T/K); temp range 316–417 K (Antoine eq., Stephenson & Malanowski 1987)
1201, 2120, 2765, 3575 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = –1.0712 – 2.5074 × 10^3/(T/K) + 6.1536·log (T/K) – 1.8763 × 10^{-2}·(T/K) + 1.0462 × 10^{-5}·$(T/K)^2$; temp range 203–624 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
272.7 (calculated-P/C, Dilling 1977)
283, 280 (calculated-P/C, recommended, Mackay & Shiu 1981)
172,2, 284, 365, 486 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
196, 320, 560 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
0.496, 0.80 (30, 40°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

Octanol/Water Partition Coefficient, log K_{OW}:
3.03 (calculated, Müller & Klein 1992)
2.62, 2.62 (30, 40°C, infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2}$ = 43 min for the evaporation from dilute aqueous solution (Dilling et al. 1975)
Evaporation $t_{1/2}$(exptl) = 42.3 min, $t_{1/2}$(calc) = 2.01 min, 48.8 min from water (Dilling 1977)
Photolysis:
Oxidation:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} < 1.0 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}, residence time > 1160 d, loss < 0.1% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
photooxidation $t_{1/2}$ = 2236–22361 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: k = 1.2 M^{-1} s^{-1} for reaction at pH 7 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991); k = 4320 M^{-1} h^{-1} for base reaction at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991); abiotic hydrolysis or dehydrohalogenation $t_{1/2}$ = 384 months (Mabey et al. 1983; quoted, Olsen & Davis 1990).
Biodegradation: aqueous aerobic $t_{1/2}$ = 672–4320 h, based on acclimated river die-away rate data for 1,1,2,2-tetrachloroethane (Mudder 1981; quoted, Howard et al. 1991), unacclimated sea water (Pearson & McConnell 1975; quoted, Howard et al. 1991) and sub-soil grab sample data for a ground water aquifer for 1,1,1-trichloroethane (Wilson et al. 1983; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 2688–17280 h, based on aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: disappearance $t_{1/2}$ = 2.4–24 h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976) residence time > 1160 d, loss < 0.1% in 1d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical with OH radical (Singh et al. 1981)

$t_{1/2}$ = 2236–22361 h, based on an estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 1.9 yr (Nimitz & Skaggs 1992).

Surface water: $t_{1/2}$ = 16–1604 h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Ground water: $t_{1/2}$ = 16–1604 h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 16–1604 h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.1.10.1
Reported aqueous solubilities of 1,1,1,2-tetrachloroethane at various temperatures

$$S/(wt\%) = 0.11968 - 7.87116 \times 10^{-4} \cdot (t/°C) + 1.42253 \times 10^{-5} \cdot (t/°C)^2 + 7.24354 \times 10^{-8} \cdot (t/°C)^3 \quad (1)$$

$$S/(wt\%) = 2.17896 - 1.3966 \times 10^{-3} \cdot (T/K) + 2.93282 \times 10^{-5} \cdot (T/K)^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982		Tse et al. 1992	
shake flask		shake flask-GC		summary of literature data		activity coefficient	
t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$
0	1200	10	1130	0	1197	20	1206
20	1090	20	1100	10	1133	30	1280
35	1150	25	1100	20	1102	35	1292
50	1250	30	1110	25	1100	40	1321
		40	1160	30	1108		
		50	1250	40	1156		
		60	1390	50	1249		
		70	1590	60	1393		
		80	1850	70	1591		
				80	1848		
				eq. 1	S/wt%		

2.

Wright et al. 1992		Horvath & Getzen 1999a	
activity coefficient		recommended, IUPAC-NIST	
t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$
20	1005	0	1200
30	1093	5	1150
40	1056	10	1110
		15	1080
		20	1070
		25	1070
		30	1080
		35	1100
		40	1130
		45	1170
		50	1230
		eq. 2	S/wt%
		temp range 273–323 K	

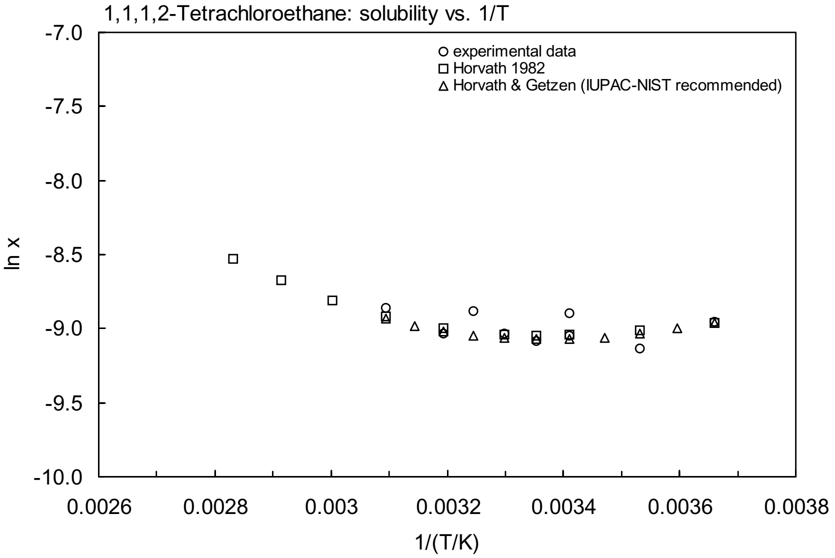


FIGURE 5.1.1.10.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

TABLE 5.1.1.10.2
Reported vapor pressures and octanol-water partition coefficients of 1,1,1,2-tetrachloroethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Vapor pressure				log K_{OW}	
Stull 1947		Dreisbach & Shrader 1949		Bhatia & Sandler 1995	
summary of literature data		ebulliometry		relative GC-RT technique	
t/°C	P/Pa	t/°C	P/Pa	t/°C	log K_{OW}
–16.3	133.3	59.31	8851	30	2.62
7.40	666.6	62.39	10114	40	2.62
19.3	1333	74.47	16500		
32.1	2666	199.69	42066	enthalpy of transfer	
46.7	5333	115.99	67881	ΔH/(kJ mol^{-1}) = –20.2.	
56.0	7999	130.2	101325		
68.0	13332			log K_{OW} = A – ΔH/2.303RT	
87.2	26664			A	1.0195.
108.2	53329			ΔH	–20.2
130.5	101325				
mp/°C	–68.7				

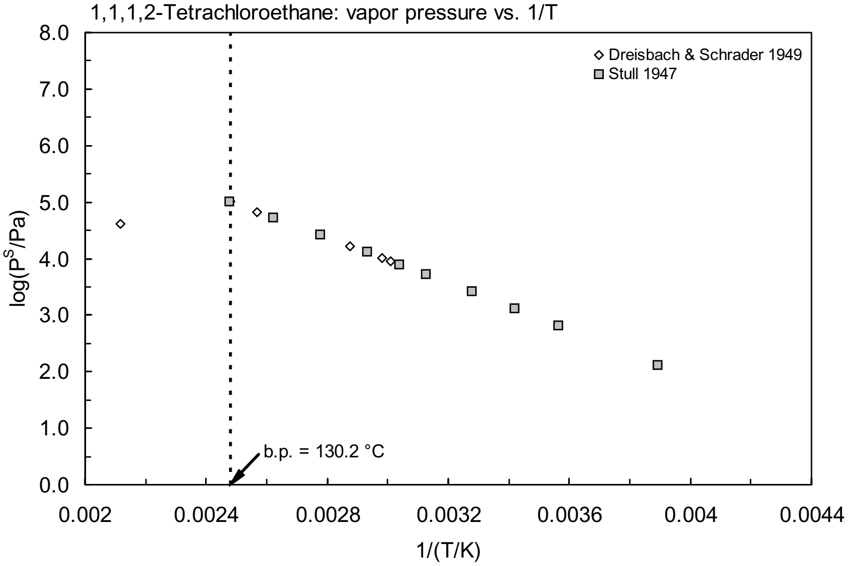


FIGURE 5.1.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

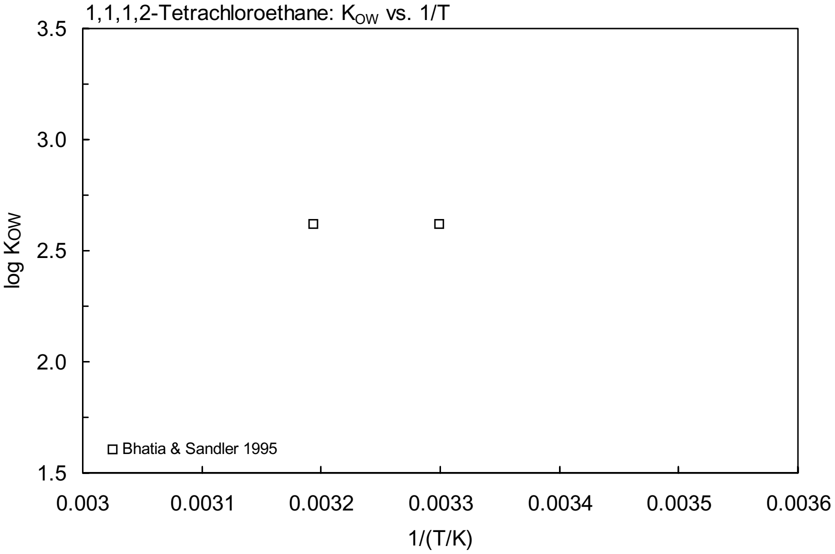
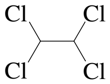


FIGURE 5.1.1.10.3 Logarithm of K_{OW} versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

5.1.1.11 1,1,2,2-Tetrachloroethane



Common Name: 1,1,2,2-Tetrachloroethane
Synonym: sym-tetrachloroethane, acetylene tetrachloride
Chemical Name: 1,1,2,2-tetrachloroethane
CAS Registry No: 79-34-5
Molecular Formula: $C_2H_2Cl_4$, $CHCl_2CHCl_2$
Molecular Weight: 167.849
Melting Point (°C):
  –42.4 (Lide 2003)
Boiling Point (°C):
  145.2 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.5953 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
  1.59449, 1.58666 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
  105.0 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)
  135.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  44.89, 36.18 (25°C, at normal boiling point, Dreisbach 1961)
  45.78, 38.65 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  2857 (volumetric method, Wright & Schaffer 1932)
  2880, 3360 (20, 55.6°C, Van Arkel & Vles 1936)
  2850 (Seidell 1940)
  2900 (data presented in graph, temp range 0–70°C, McGovern 1943)
  2960* (shake flask-GC, measured range 10–80°C, Walraevens et al. 1974)
  $\log [S/(mol/L)] = 2070/(T/K) - 16.316 + 0.0222\cdot(T/K)$, temp range 283–353 K (Walraevens et al. 1974)
  3790, 3220, 3210 (3, 20, 34°C, shake flask-GC, Chiou & Freed 1977)
  3000 (literature average, Dilling 1977)
  3230 (shake flask-GC, Chiou et al. 1979)
  3041 (37°C, shake flask-GC, Sato & Nakijima 1979)
  2880 (20°C, recommended, Sørensen & Arit 1979)
  2970 (shake flask-LSC, Banerjee et al. 1980)
  2960 (23.5°C, elution chromatography, Schwartz 1980)
  3850* (20°C, elution chromatography, measured range 10–30°C, Schwarz & Miller 1980)
  2985 (shake flask-LSC, Veith et al. 1980)
  2962* (summary of literature data, temp range 0–80°C, Horvath 1982)
  866.4 (calculated-UNIFAC activity coeff., Arbuckle 1983)
  2915 (30°C, headspace-GC, McNally & Grob 1984)
  2985 (calculated-UNIFAC activity coeff., Banerjee 1985)
  2870 (20°C, selected, Riddick et al. 1986)
  2355, 2695, 3008 (20, 35, 50°C, infinite dilution activity coeff. γ^∞-GC, Barr & Newsham 1987)
  2910* (20°C, shake flask-GC/TC, measured range 0–90.8°C, Stephenson 1992)
  2481, 2503, 2917, 3008 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
  778, 918, 994, 1074 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)

2422, 3140, 2612 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
2570 (20°C, activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
2830* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 4.87975 – 3.0937 × 10^{-3}·(T/K) + 5.20513 × 10^{-5}·$(T/K)^2$, temp range 276–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
827* (static method, extrapolated, measured range 31.1–146.7°C, Nelson 1930)
log (P/mmHg) = 8.06938 – 2167.83/(T/K); temp range 31.1–146.7°C (static method, Nelson 1930)
850* (Antoine eq. regression, temp range 65–243.5°C, Stull 1947)
560* (Ramsay-Young method, measured range 25–130°C, Matthews et al. 1950)
793 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.98240 – 1465.1/(211.0 + t/°C); temp range 55–191°C (Antoine eq. for liquid state, Dreisbach 1961)
851 (interpolated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9917.1/(T/K)] + 8.072583; temp range –3.8 to 146°C (Antoine eq., Weast 1972–73)
582 (calculated-Antoine eq., Boublik et al. 1973)
log (P/kPa) = 6.63168 – 1228.062/(179.972 + t/°C); temp range 25–120°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
867 (literature average, Dilling 1977)
585 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.77919 – 1240.857/(181.401 + t/°C); temp range 25–130°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
2133 (McNally & Grob 1984)
log (P/mmHg) = 6.6317 – 1228.1/(279.9 + t/°C); temp range 25–130°C (Antoine eq., Dean 1985, 1992)
793 (selected, Riddick et al. 1986)
log (P/kPa) = 6.1295 – 1444.3/(205.1 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
793 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.1073 – 1465.1/(–62.15 + T/K); temp range 328–464 K (Antoine eq-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.98931 –1365.692/(–76.476 + T/K); temp range 377–419 K (Antoine eq.-II, Stephenson & Malanowski 1987)
440, 848, 1154, 2550(20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 56.2356 – 4.4615 × 10^3/(T/K) –1 6.556·log (T/K) – 3.5724 × 10^{-10}·(T/K) + 4.0425 × 10^{-6}·$(T/K)^2$; temp range 229–645 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
46.2 (exptl. 1/K_{AW} (C_W/C_A), Hine & Mookerjee 1975)
47.1 (calculated-P/C, Dilling 1977)
35.38* (22.0°C, equilibrium cell-GC, measured range 11.0–27.2°C, Leighton & Calo 1981)
48.5, 48.0 (calculated-P/C, recommended, Mackay & Shiu 1981)
25.3* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 1.726 – 2810/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
38.5 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
33.45 (computed value, Yaws et al. 1991)
30.4, 50.7, 60.8, 91.2 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
40.3, 57.06, 120 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
34.4 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
34.12 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 2.493 – 1255/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
2.56 (calculated as per Tute 1971, Callahan et al. 1979)
2.39 (shake flask-LSC, Banerjee et al. 1980)

2.39	(shake flask-LSC, Veith et al. 1980)
2.79, 2.84	(calculated-UNIFAC with octanol and water mutual solubility considered, calculated-UNIFAC with octanol and water mutual solubility not considered; Arbuckle 1983)
2.39	(calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
2.93	(recommended, Sangster 1993)
2.39	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.9–1.0	(bluegill sunfish, Barrows et al. 1980; Kawasaki 1980)
0.90	(bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
1.96	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
0.91	(fathead minnow, Veith & Kosian 1982)
2.03	(calculated-K_{OW}, McCarty et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

1.66	(soil, equilibrium sorption isotherm, Chiou et al. 1979)
1.90	(silt loam, quoted from Chiou et al. 1979; Karickhoff 1981; Howard 1990)
2.00, 1.80. 1.87	(estimated-K_{OW}, estimated-S and mp, estimated-S, Karickhoff 1981)
2.07	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)
3.60	(soil, calculated-universal solvation model; Winget et al. 2000)

Sorption Partition Coefficient, log K_{OM}:

1.66, 1.90	(quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental $t_{1/2}$ = 56 min for initial concentration of 1 mg/L when stirred at 200 rpm in water at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

Evaporation $t_{1/2}$(exptl) = 55.2 min, $t_{1/2}$(calc) = 12.0 min, 40.5 min from water (Dilling 1977);

estimated $t_{1/2}$ ~ 6.3 h for a model river of 1 m deep flowing at 1 m/s with a wind speed of 3 m/s, based on calculated Henry's law constant (Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2}$ ~ 3.5 d for a model pond was based on the effect of adsorption (USEPA 1987; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k << 360 M^{-1} h^{-1} for singlet oxygen and k = 2.0 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

k_{OH} < 1.0×10^{-14} cm^3 $molecule^{-1}$ s^{-1}, estimated as toxic chemical residence time > 1160 d, loss < 0.1% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2}$ = 213–2131 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: k = 1.2×10^{-7} h^{-1} at 25°C and pH 7 (estimated, Mabey et al. 1982);

$t_{1/2}$(abiotic) or $t_{1/2}$(dehydrohalogenation) = 10 months (Mabey et al. 1983; quoted, Olsen & Davis 1990)

$t_{1/2}$(abiotic) = 3.3 months (Cooper et al. 1987; quoted, Olsen & Davis 1990);

k = 2.3×10^7 M^{-1} yr^{-1} at pH 9 and 25°C with $t_{1/2}$ = 1.1 d in alkaline soil, and k = 111 d at pH 7 (Kollig et al. 1987; quoted, Howard 1990)

k = 1.8 M^{-1} s^{-1} for base-catalyzed reaction at 25°C and pH 7 with $t_{1/2}$ = 45 d;; k = 6480 M^{-1} h^{-1} for base reaction at pH 9 and 25°C; k = $(27.6 \pm 4.0) \times 10^{-8}$ s^{-1} in sediment with 61% conversion (Haag & Mill 1988)

Biodegradation: k = $(7.3 \pm 0.1) \times 10^{-5}$ min^{-1} with $t_{1/2}$ = 6.6 d in sediment-water sample (Jafvert & Wolfe 1987)

$t_{1/2}$(abiotic) > 800 d for the reaction with photochemically produced hydroxyl radical (Singh et al. 1981; quoted, Howard 1990)

$t_{1/2}$(aq. aerobic) = 672–4320 h, based on acclimated river die-away rate data (Mudder 1981; quoted, Howard et al. 1991)

$t_{½}$(aq. anaerobic) = 168–672 h, based on anaerobic sediment grab sample data (Jafvert & Wolfe 1987) and anaerobic screening test data (Hallen et al. 1986; quoted, Howard et al. 1991).

Biotransformation: estimated rate constant of 3×10^{-12} mL cell^{-1} h^{-1} for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

k_1 = 13.2 h^{-1} (flagfish, calculated-BCF × k_2, McCarty et al. 1992)

k_2 = 0.123 h^{-1} (flagfish, estimated-one compartment first-order kinetic, McCarty et al. 1992)

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976); estimated as toxic chemical residence time > 1160 d, loss < 0.1% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{½}$ = 213–2131 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

estimated tropospheric lifetime of 0.09 yr (Nimitz & Skaggs 1992).

Surface water: $t_{½}$ = 6.6 d in sediment-water sample (Jafvert & Wolfe 1987);

$t_{½}$ = 45 d at pH 7 and 25°C, based on based-catalyzed hydrolysis rate constant (Haag & Mill 1988);

$t_{½}$ = 10.7–1056 h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Ground water: $t_{½}$ = 10.7–1056 h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Sediment: $t_{½}$ = 6.6 d in Bar-H sediment-water sample (Jafvert & Wolfe 1987);

measured $t_{½}$ = 29 d at 25°C, based on neutral and base-catalyzed hydrolysis rates studies in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil: $t_{½}$ < 10 d (Ryan et al. 1988);

$t_{½}$ = 10.7–1056 h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Biota: $t_{½}$ < 1 d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{½}$ < 10 d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.11.1
Reported aqueous solubilities of 1,1,2,2-tetrachloroethane at various temperatures

$$\log S/(\text{mol/L}) = -15.316 + 2070/(T/K) + B(T/K) \quad (1)$$

$$S/(\text{wt\%}) = 0.32934 - 2.10434 \times 10^{-3}\cdot(t/°C) + 2.54796 \times 10^{-5}\cdot(t/°C)^2 + 1.86126 \times 10^{-7}\cdot(t/°C)^3 \quad (2)$$

$$S/(\text{wt\%}) = 4.87975 - 3.0937 \times 10^{-3}\cdot(T/K) + 5.20513 \times 10^{-5}\cdot(T/K)^2 \quad (3)$$

1.

Walraevens et al. 1974		Schwarz & Miller 1980		Horvath 1982		Barr & Newsham 1987	
shake flask-GC		elution chromatography		summary of literature data		activity coefficient	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
10	3200	10	3720	0	3299	20	2235
20	3010	20	3850	10	3116	35	2595
25	2960	30	3670	20	2995	50	3008
30	2940			25	2962		
40	2980			30	2948		
50	3120			40	2984		
60	3360			50	3118		
70	3710			60	3356		
80	4200			70	3713		
				80	4199		
eq. 1	S/(mol/L)						
A	15.316						
B	0.0222			eq. 2	S/wt%		

TABLE 5.1.1.11.1 (*Continued*)

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999a	
shake flask-GC		activity coefficient		activity coefficient		recommended, IUPAC-NIST	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
0	3170	20	2481	20	2422	5	3020
9.5	2900	30	2503	30	3140	10	2830
20	2910	35	2917	40	2612	15	2870
29.7	2920	40	3008			25	2840
39.6	3010					30	2830
50.1	3160					35	2850
61	3570					40	2890
70.5	3850					45	3060
80.6	4250					50	3160
90.8	4740						
						eq. 3	S/wt%
						temp range 276–323 K	

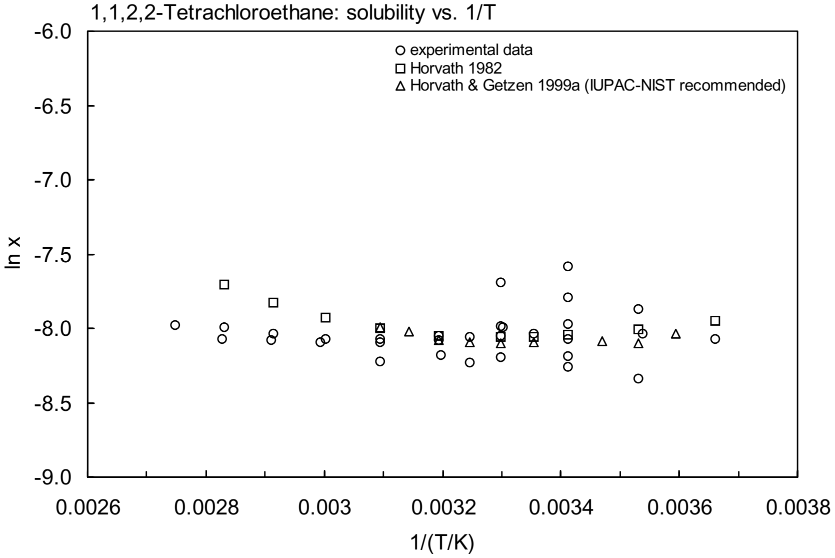


FIGURE 5.1.1.11.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

TABLE 5.1.1.11.2
Reported vapor pressures of 1,1,2,2-tetrachloroethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Nelson 1930		Stull 1947		Matthews et al. 1950	
static method		summary of literature data		Ramsay-Young method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
31.1	1000	–3.80	133.3	25.0	560
34.6	1067	20.7	666.6	30.0	667
39.3	1533	33.0	1333	35.0	1080
44.3	2200	46.2	2666	40.0	1493
50.4	3120	60.8	5333	45.0	2000
57.8	4253	70.0	7999	50.0	2680
64.6	5893	83.2	13332	55.0	3480
72.3	8293	102.2	26664	60.0	4440
79.0	10879	124.0	53329	65.0	5626
85.0	13865	145.9	101325	70.0	6933
89.9	16785			75.0	8533
94.9	20438	mp/°C	–36	80.0	10666
99.9	24611			85.0	13066
105	29851			90.0	16079
109.1	34770			95.0	19532
114.9	41730			100	23665
119.9	47703			105	28331
120.1	48569			110	33130
124.5	54865			115	38930
130.4	66328			120	45663
135.2	92139			135	53329
141.5	102285			130	62795
146.7	106938				
20	626.6*			bp/K	420.4
25	826.6*			ΔH_V = 38.42 kJ/mol at bp	
				Kirchhoff, Rankine, Dupre eq.	
eq. 1	P/mmHg			eq. 4	P/mmHg
A	8.08938			A	35.117
B	2167.83			B	3646
				C	8.981

*extrapolated

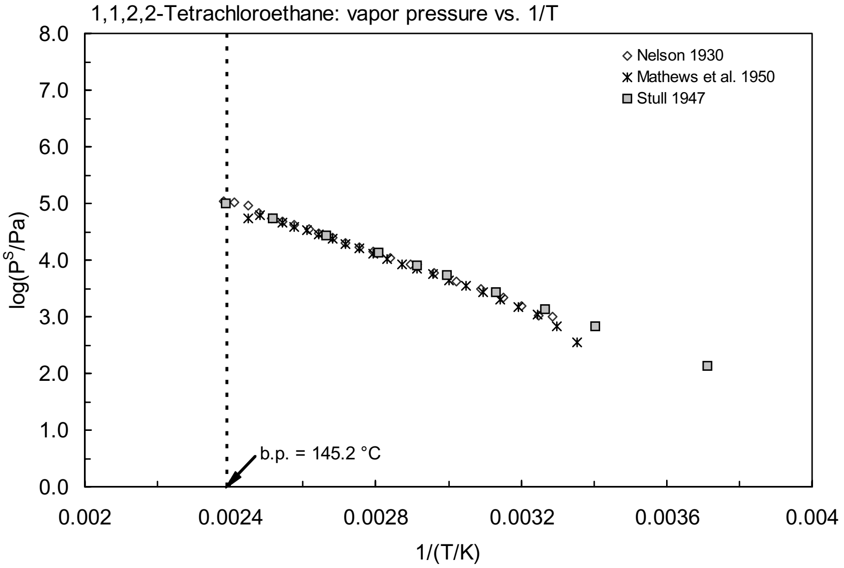


FIGURE 5.1.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

TABLE 5.1.1.11.3
Reported Henry's law constants of 1,1,2,2-tetrachloroethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$ (4)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)
$\log K_{AW} = A - B/(T/K)$ (1a)
$\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$ (4a)

Leighton & Calo 1981		Ashworth et al. 1988		Tse et al. 1992		Wright et al. 1992	
equilibrium cell-GC		EPICS-GC		activity coefficient		activity coefficient	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
11.0	19.95	10	33.44	20	30.4	20	40.3
13.0	22.83	15	20.27	30	50.7	30	57.06
21.0	31.06	20	73.97	35	60.8	40	120
22.0	35.38	25	25.33	40	91.2		
27.2	38.19	30	70.93				
eq. 3	H/atm	eq. 4a	H/(atm m^3/mol)				
A	14.91	A	1.726				
B	3547	B	2810				

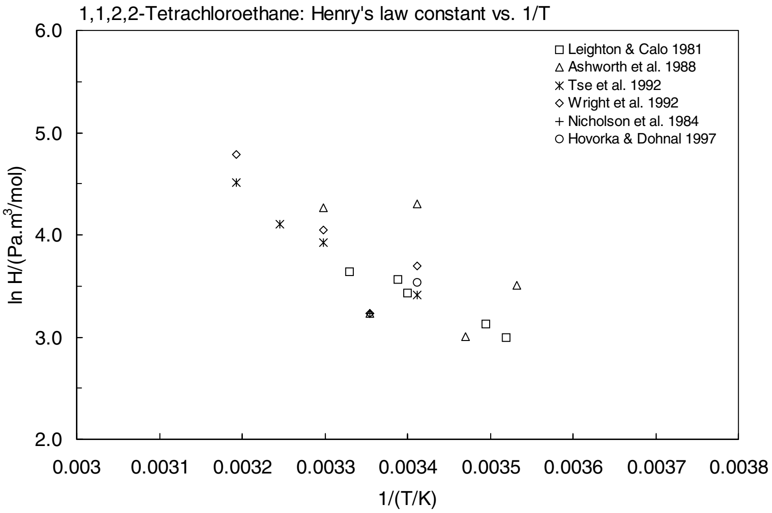
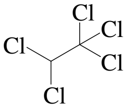


FIGURE 5.1.1.11.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

5.1.1.12 Pentachloroethane



Common Name: Pentachloroethane
Synonym: 1,1,1,2,2-pentachloroethane, pentalin
Chemical Name: pentachloroethane
CAS Registry No: 76-01-7
Molecular Formula: C_2HCl_5, $CHCl_2CCl_3$
Molecular Weight: 202.294
Melting Point (°C):
–28.78 (Lide 2003)
Boiling Point (°C):
162.0 (Horvath 1982; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 20°C):
1.6796 (Horvath 1982; Weast 1982–83)
1.6808, 1.6732 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
120 (calculated-density, Abernethy et al. 1988)
156.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
40.79, 36.941 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.34 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
345 (volumetric method, Wright & Schaffer 1932)
470 (20°C, shake flask, Van Arkel & Vles 1936)
463 (Seidell 1940)
500 (data presented in graph, temp range 0–70°C, McGovern 1943)
500* (shake flask-GC, temp range 10–80°C, Walraevens et al. 1974)
$\log [S/(\text{mol dm}^{-3})] = 2070/(T/K) - 16.412 + 0.0230\cdot(T/K)$; temp range 283–353 K (Walraevens et al. 1974)
480 (literature average, Dilling et al. 1975; Dilling 1977)
776 (shake flask-LSC, Veith et al. 1980)
500* (summary of literature data, temp range 0–80°C, Horvath 1982)
500 (Dean 1985; Riddick et al. 1986)
470, 490 (20°C, 25°C, recommended, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):
467* (25.1°C, static method, measured range 25.1–162.2°C, Nelson 1930)
$\log (P/\text{mmHg}) = 7.80304 - 2129.6/(T/K)$; temp range 25.1–162.2°C (static method, Nelson 1930)
596* (Antoine eq. regression, temp range 1.0–160.5°C, Stull 1947)
596 (calculated-Antoine eq., Weast 1972–73)
$\log (P/\text{mmHg}) = [-0.2185 \times 9800.1/(T/K)] + 7.832202$; temp range 1.0–160.6°C (Antoine eq., Weast 1972–73)
465 (calculated-Antoine eq., Boublik et al. 1973)
$\log (P/\text{mmHg}) = 6.74011 - 1378.096/(197.367 + t/°C)$; temp range 25.1–162°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
600 (literature average, Dilling 1977)
453, 800 (20°C, 30°C, Verschueren 1983)

467 (calculated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 5.92765 - 1419.719/(202.285 + t/°C)$; temp range 25.1–162°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (P/mmHg) = 6.740 - 1378/(197 + t/°C)$, temp range: 25–162°C (Antoine eq., Dean 1985, 1992)
590 (selected, Riddick et al. 1986)
$\log (P/kPa) = 5.7199 - 1295.67/(188.96 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
625 (calculated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.69025 - 1982.65/(-10.577 + T/K)$; temp range 274–434 K (Antoine eq., Stephenson & Malanowski 1987)
467, 453 (quoted, calculated-UNIFAC, Banerjee et al. 1990)
$\log (P/mmHg) = 72.1134 - 4.6522 \times 10^3/(T/K) - 23.777 \cdot \log (T/K) + 9.6908 \times 10^{-3} \cdot (T/K) - 3.3886 \times 10^{-13} \cdot (T/K)^2$; temp range 244–665 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
247.9 (exptl $-1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975)
247.9 (calculated-P/C, Dilling 1977)
96.44 (calculated-QSAR, Nirmalakhandan & Speece 1988)
196.5 (calculated-P/C, Howard 1990)
188.9, 53.73 (quoted, calculated-bond contribution method, Meylan & Howard 1991)
183.9 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
2.89 (shake flask-LSC, Veith et al. 1980)
3.05 (HPLC-RT correlation, McDuffie 1981; quoted, Sangster 1993)
3.22 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.826 (bluegill sunfish, Barrows et al. 1980)
1.83 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
1.78 (fathead minnow, Veith & Kosian 1982)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant, k and Half-Lives, $t_{1/2}$:
Volatilization: estimated experimental $t_{1/2}$ = 48 min for 1 mg/L aqueous solution when stirred at 200 rpm at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975)
Evaporation $t_{1/2}$(exptl) = 46.5 min, $t_{1/2}$(calc) = 2.3 min, 32 min from water (Dilling 1977)
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 1.93×10^{-14} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = 2.33×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);
estimated tropospheric lifetime of 0.58 h (Nimitz & Skaggs 1992).
Surface water:
Ground water:
Sediment:
Soil:
Biota: $t_{1/2}$ < 1 d in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 5.1.1.12.1
Reported aqueous solubilities and vapor pressures of pentachloroethane at various temperatures

$$S/(\mathrm{wt}\%) = 5.41068 \times 10^{-2} - 2.81268 \times 10^{-4}\cdot(t/°C) + 3.41333 \times 10^{-6}\cdot(t/°C)^2 + 4.76167 \times 10^{-8}\cdot(t/°C)^3 \quad (1)$$

$$\log S = A/(T/K) - B + C\cdot(T/K) \quad (2)$$

Aqueous solubility				Vapor pressure			
Walraevans et al. 1974		Horvath 1982		Nelson 1930		Stull 1947	
shake flask-GC		summary of literature data		static method		summary of literature data	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	P/Pa	t/°C	P/Pa
10	520	0	541.1	25.1	467	1.0	133.3
20	500	10	516.8	41.1	1733	27.2	666.6
25	500	20	502.3	50.0	2133	39.8	1333
30	500	25	499.5	55.0	2666	53.9	2666
40	510	30	500.3	65.0	4453	69.9	5333
50	550	40	513.6	69.0	4986	80.0	7999
60	600	50	545.3	75.0	6573	93.5	13332
70	670	60	598.0	80.0	7973	114.0	26664
80	780	70	674.8	88.2	10959	137.2	53329
		80	778.3	95.7	14212	160.5	101325
eq. 2	S/(mol/L)			100.2	16732		
A	2070	eq.1	S/wt%	105.0	19852	mp/°C	57
B	16.412			110.0	23771		
C	0.0230			115.6	28491		
				119.9	33064		
				124.9	39170		
				125.6	39957		
				128.7	43876		
				132.4	49049		
				134.6	50249		
				139.4	59555		
				145.3	70741		
				151.3	80660		
				157.3	94859		
				162.2	108137		

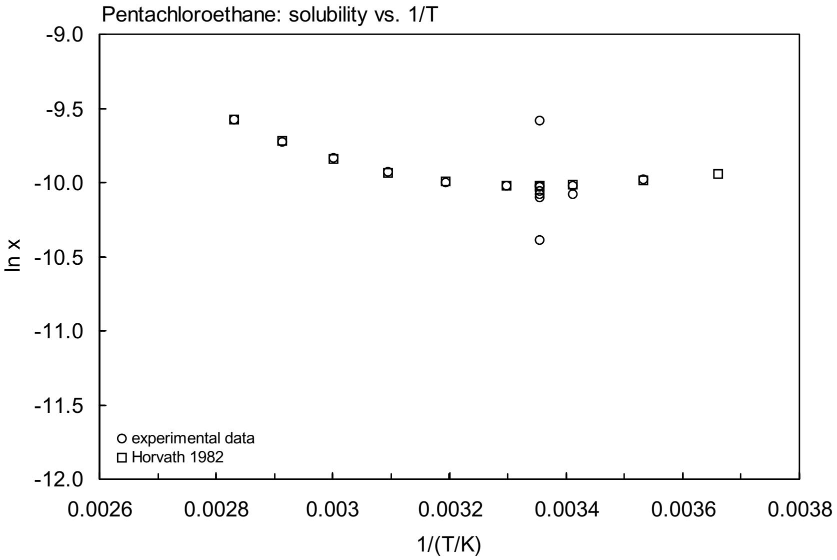


FIGURE 5.1.1.12.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for pentachloroethane.

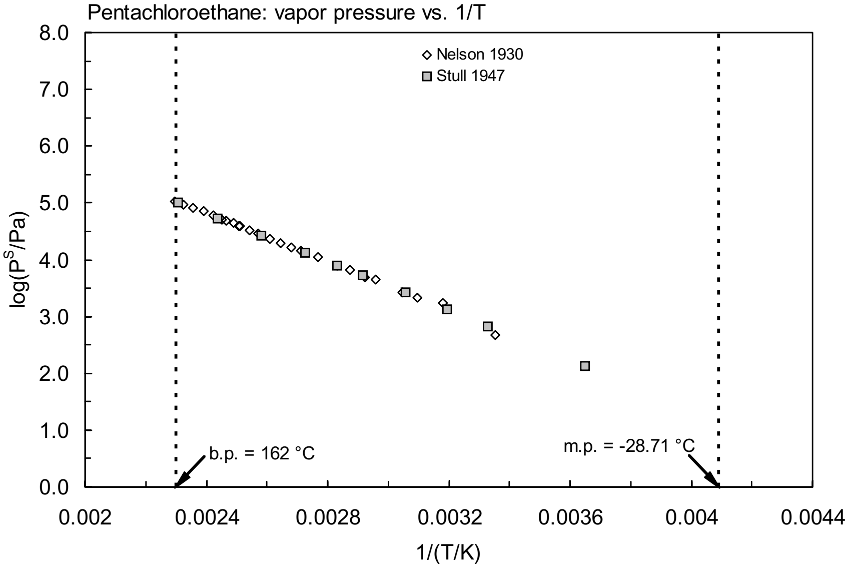
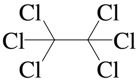


FIGURE 5.1.1.12.2 Logarithm of vapor pressure versus reciprocal temperature for pentachloroethane.

5.1.1.13 Hexachloroethane



Common Name: Hexachloroethane
Synonym: carbon hexachloride, perchloroethane, phenohep, HCE
Chemical Name: hexachloroethane
CAS Registry No: 67-72-1
Molecular Formula: C_2Cl_6, CCl_3CCl_3
Molecular Weight: 236.739
Melting Point (°C):
186.8 (triple point) (Lide 2003)
Boiling Point (°C):
184.7 (sublimation point) (Lide 2003)
Density (g/cm^3 at 20°C):
2.091 (McGovern 1943; Horvath 1982; Weast 1982–83; Dean 1985)
Molar Volume (cm^3/mol):
113 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)
177.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
50 (22.3°C, shake flask, Van Arkel & Vles 1936)
50 (22.3°C, McGovern 1943)
27.2 (shake flask-LSC, Veith et al. 1980)
50 (22.3°C, recommended, Horvath 1982)
77.1 (20°C, EPICS-LSC, Munz & Roberts 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
42.7* (gas saturation method, extrapolated, measured range 31–55°C, Nelson 1930)
75.4* (extrapolated-Antoine eq. regression, temp range 32.7–186.5°C, Stull 1947)
$\log (P/\text{mmHg}) = [-0.2185 \times 11711.3/(T/K)] + 8.440623$; temp range 32.7–185.6°C (Antoine eq., Weast 1972–73)
49.5 (calculated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_S/\text{kPa}) = 7.9015 - 3077/(T/K)$; temp range 317–345 K (Antoine eq.-I, solid, rhombic, Stephenson & Malanowski 1987)
$\log (P_S/\text{kPa}) = 7.856 - 2677/(T/K)$; temp range 345–460 K (Antoine eq.-II, solid, cubic, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.6075 - 2103.6/(T/K)$; temp range 460–513 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = -366.2243 + 6.67893 \times 10^3/(T/K) + 155.63 \cdot \log (T/K) - 0.15563 \cdot (T/K) + 5.56 \times 10^{-5} \cdot (T/K)^2$; temp range 306–698 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
231.3 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
123.9 (calculated-P/C, Dilling 1977)
285* (20°C, EPICS-LSC, measured range 10–30°C, Munz 1985)
$\log K_{AW} = 6.982 - 2320/(T/K)$, temp range 10–30°C (EPICS-LSC measurements, Munz & Roberts 1987)

846*	(EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm·m^3/mol)] = 3.744 – 2550/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

253.3	(20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
226.7	(computed value, Yaws et al. 1991)
285	(20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 6.982 – 2320/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

4.14	(20°C, shake flask-GC, both phases, Chiou et al. 1977)
3.82	(HPLC-k′ correlation, Könemann et al. 1979)
3.93	(shake flask-LSC, Veith et al. 1980)
4.05	(RP-HPLC-RT correlation, Veith et al. 1980)
4.04	(HPLC-RT correlation, McDuffie 1981)
4.14	(recommended, Sangster 1993)
4.14	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

4.47	(calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

0.92–3.23	(calculated-K_{OW}, Veith et al. 1979,1980)
2.143	(bluegill sunfish, Barrows et al. 1980)
2.14	(bluegill sunfish, Veith et al. 1980)
3.83	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
2.14	(bluegill sunfish, Veith & Kosian 1982)
2.85	(fathead minnow, Veith & Kosian 1982)
4.57	(calculated-K_{OW}, Thomann 1989)

Sorption Partition Coefficient, log K_{OC}:

4.3	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental $t_{1/2}$ = 40–45 min from dilute aqueous solution in open container of depth 65mm and stirring at 200 rpm (Dilling et al. 1975)

Evaporation $t_{1/2}$(exptl) = 28.0 min, $t_{1/2}$(calc) = 4.5 min, 24.5 min from water (Dilling 1977)

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} < 1.0 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1}, estimated residence time > 11600 d, loss ≈0.0% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2}$ > 7.3–73 yr, based on estimated maximum rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: not significant, based on hydrolysis studies after 13 d at 85°C and pH 3, 7, and 11 (Ellington et al. 1987; quoted, Howard et al. 1991)

Biodegradation:

k = (5.0 ± 0.34) × 10^{-2} min^{-1} in Bar-H sediment-water slurry, k = (2.0 ± 0.17) × 10^{-2} min^{-1} in Beaver Dam sediment-water slurry, k = (2.6 ± 0.2) × 10^{-2} min^{-1} in Hickory Hill sediment-water slurry, k = (1.9 ± 0.16) × 10^{-2} min^{-1} in Memorial Park sediment-water slurry and k = (1.9 ± 0.1) × 10^{-2} min^{-1} with $t_{1/2}$ = 36 min in anoxic Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

$t_{1/2}$(aq. aerobic) = 672 h–4320 h, based on aqueous screening studies (Howard et al. 1991)

$t_{1/2}$(aq. anaerobic) = 2688–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}$(aerobic) = 28 d, $t_{1/2}$(anaerobic) = 110 d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of 1 × 10^{-10} ml cell^{-1} h^{-1} for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} > 10$ d for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} > 7.3$–73 yr, based on estimated maximum rate constant for reaction with hydroxyl radical (Singh et al. 1980; quoted, Howard et al. 1991);

residence time > 11600 d, loss ≈ 0.0 in 1d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical K for the reaction with OH radical (Singh et al. 1981)

Surface water: $t_{1/2} = 36$ min in anoxic sediment-water suspension (Jafvert & Wolfe 1987);

$t_{1/2} = 672$–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}$(aerobic) = 28 d, $t_{1/2}$(anaerobic) = 110 d in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2} = 1344$–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: disappearance $k = (5.0 \pm 0.34) \times 10^{-2}\ \text{min}^{-1}$ in Bar-H sediment-water slurry, $k = (2.0 \pm 0.17) \times 10^{-2}\ \text{min}^{-1}$ in Beaver Dam sediment-water slurry, $k = (2.6 \pm 0.2) \times 10^{-2}\ \text{min}^{-1}$ in Hickory Hill sediment-water slurry, $k = (1.9 \pm 0.16) \times 10^{-2}\ \text{min}^{-1}$ in Memorial Park sediment-water slurry and $k = (1.9 \pm 0.1) \times 10^{-2}\ \text{min}^{-1}$ with $t_{1/2} = 36$ min in Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

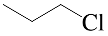
Soil: $t_{1/2} = 672$–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980)

TABLE 5.1.1.13.1
Reported vapor pressures and Henry's law constant of hexachloroethane at various temperatures

Vapor pressure				Henry's law constant			
Nelson 1930		Stull 1947		Ashworth et al. 1988		Munz 1985	
gas saturation		summary of literature data		EPICS-GC		EPICS-LSC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
31	73.3	32.7	133.3	10	601	10	74.2
35	93.3	49.8	666.6	15	566.4	20	285
40	133.3	73.5	1333	20	598.8	30	537
45	198.7	87.6	2666	25	846.1		
50	282.6	102.3	5333	30	1044		
55	390.6	112.0	7999				
		124.2	13332	ln [H/(atm·m^3/mol)] = A – B/(T/K)			
		143.1	26664	A	3.744		
		163.8	53332	B	2550		
		185.6	101325				

5.1.1.14 1-Chloropropane (*n*-Propyl chloride)



Common Name: 1-Chloropropane
Synonym: *n*-Propyl chloride, propyl chloride
Chemical Name: 1-chloropropane, *n*-Propyl chloride, propyl chloride
CAS Registry No: 540-54-5
Molecular Formula: $CH_3CH_2CH_2Cl$
Molecular Weight: 78.541
Melting Point (°C):
–122.9 (Lide 2003)
Boiling Point (°C):
46.5 (Lide 2003)
Density (g/cm^3 at 20°C):
0.8909 (Dreisbach 1961; Horvath 1982)
0.8899, 0.8830 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
88.3 (20°C, calculated-density)
94.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
28.48, 27.25 (25°C, normal bp, Dreisbach 1961)
28.50, 27.24 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
5.544 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
2720* (20°C, measured range 0–30°C, volumetric method, Rex 1906)
2500 (Wright & Schaffer 1932)
2772 (30°C, shake flask, Van Arkel & Vles 1936)
2334 (Seidell 1941)
2333 (20°C, Saracco & Spaccamela Marchetti 1958)
2700 (20°C, Verschueren 1983)
2651* (summary of literature data, Horvath 1982)
2710 (20°C, quoted, Riddick et al. 1986)
2500* (reported value of IUPAC-NIST Solubility Data Series, temp range 0–37°C, Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
37360, 55240 (20°C, 30°C, Rex 1906)
46500* (interpolated-Antoine eq. regression, temp range –68.3 to 36.5°C, Stull 1947)
46000 (calculated-Antoine eq., Dreisbach 1961)
$\log (P/mmHg) = 6.93111 - 1121.123/(230.2 + t/°C)$; temp range –25 to 88°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = 6.93111 - 1121.123/(230.20 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
40517* (21.8°C, differential thermal analysis, measured range –25.1 to 47.1°C, Kemme & Kreps 1969)
$\log (P/mmHg) = [-0.2185 \times 7485.7/(T/K)] + 8.028733$; temp range –63.8 to 46.4°C (Antoine eq., Weast 1972–73)
$\log (P/kPa) = 6.07206 - 1120.381/(229.061 + t/°C)$; temp range –25.1 to 47.1°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)
$\log (P/mmHg) = 6.92648 - 1110.19/(227.94 + t/°C)$; temp range –25 to 47°C (Antoine eq., Dean 1985, 1992)

45920 (selected, Riddick et al. 1986)
$\log (P/kPa) = 6.07655 - 1125.09/(229.86 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
46060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.09145 - 1126.383/(-43.78 + T/K)$; temp range 248–320 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = 32.3325 - 2.485 \times 10^3/(T/K) - 8.8052\cdot\log (T/K) + 8.9119 \times 10^{-11}\cdot(T/K) + 3.6803 \times 10^{-6}\cdot(T/K)^2$; temp range 150–503 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

1341	(calculated-P/C, using Hine & Mookerjee 1975 data)
1600	(calculated-QSAR, Nirmalakhandan & Speece 1988)
1091	(computed value, Yaws et al. 1991)
1450	(γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

2.04	(shake flask, Log P Database, Hansch & Leo 1987)
2.04	(recommended, Sangster 1989)
2.04	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

2.24	(head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 5.1.1.14.1
Reported aqueous solubilities of 1-chloropropane at various temperatures

$$S/(wt\%) = 0.3746 - 0.007725\cdot(t/°C) + 1.05001 \times 10^{-6}\cdot(t/°C)^2 + 1.14998 \times 10^{-6}\cdot(t/°C)^3 \quad (1)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		reported, IUPAC-NIST	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	3760	0	3746	0	3750
10	3230	10	3090	10	3220
20	2720	20	2713	12.5	2320
30	2770	25	2651	20	2710
		30	2684	25	2500
				30	2760
		eq. 1	S/wt%	30	2770
				37	2440

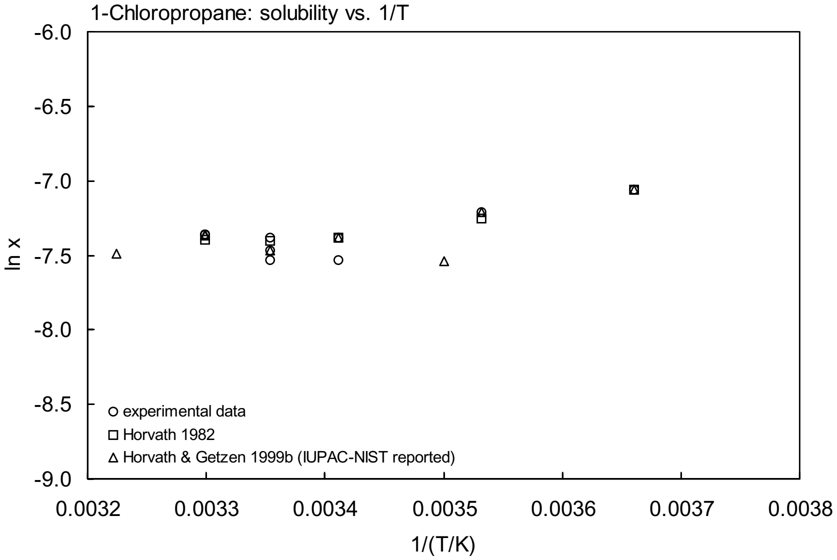


FIGURE 5.1.1.14.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1-chloropropane.

TABLE 5.1.1.14.2
Reported vapor pressures of 1-chloropropane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		**Kemme & Kreps 1969**	
summary of literature data		**differential thermal analysis**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**
–63.8	133.3	–25.1	3840
–50.0	666.6	–19.6	5320
–41.0	1333	–13.7	7386
–31.0	2666	–6.90	10599
–19.5	5333	1.20	16065
–12,1	7999	12.1	26691
–2.50	13332	21.8	40517
12.1	26664	34.9	67194
29.4	53329	47.1	103458
46.4	101325		
		eq. 2	P/mmHg
mp/°C	–117	A	8.18894
		B	1690.864
		C	221.346

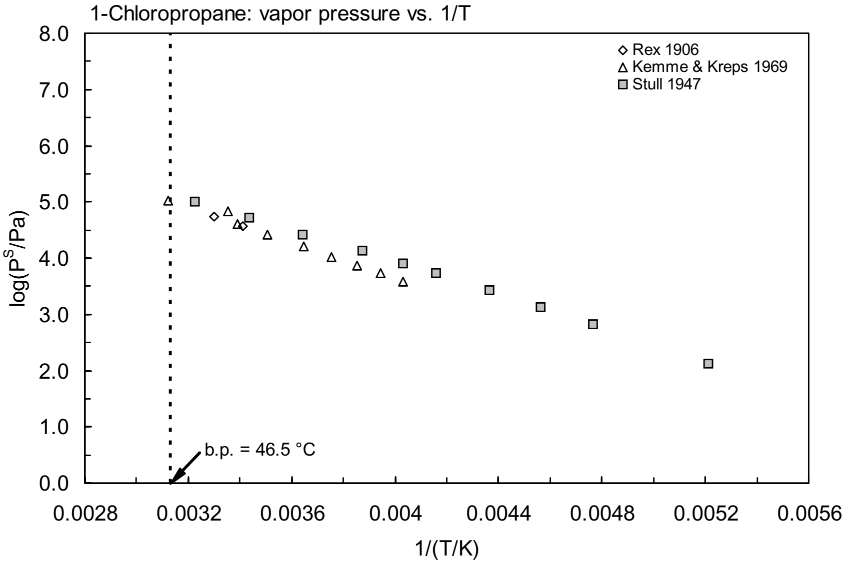
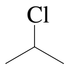


FIGURE 5.1.1.14.2 Logarithm of vapor pressure versus reciprocal temperature for 1-chloropropane.

5.1.1.15 2-Chloropropane



Common Name: 2-Chloropropane
Synonym: isopropyl chloride
Chemical Name: 2-chloropropane, isopropyl chloride
CAS Registry No: 75-29-6
Molecular Formula: C_3H_7Cl, $CH_3CHClCH_3$
Molecular Weight: 78.541
Melting Point (°C):
–117.18 (Lide 2003)
Boiling Point (°C):
35.7 (Lide 2003)
Density (g/cm^3 at 20°C):
0.8626, 0.8560 (20°C, 25°C, Dreisbach 1959)
0.8617, 0.8563 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm^3/mol):
91.2 (20°C, calculated from density)
94.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
26.86, 26.26 (25°C, normal bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
7.39 (calculated, Dreisbach 1959)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
3050* (20°C, measured range 0–30°C, volumetric method, Rex 1906)
3444 (shake flask, Fühner 1924)
3056 (Seidell 1940)
3000 (Seidell 1941)
2950 (selected exptl., Horvath 1982)
3400 (Dean 1985)
3040* (20°C, tentative values, temp range 0–30°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
58050, 83940 (20°C, 30°C, Rex 1906)
53329* (18.1°C, summary of literature data, temp range –78.8 to 36.5°C, Stull 1947)
70580 (calculated-Antoine eq., Dreisbach 1959)
$\log (P/\text{mmHg}) = 6.96540 - 1081.6/(230 + t/°C)$; temp range –32 to 90°C (Antoine eq. for liquid state, Dreisbach 1959)
68700 (interpolated-Antoine eq., Dreisbach 1961)
$\log (P/\text{mmHg}) = 6.91997 - 1081.4/(232 + t/°C)$; temp range –33 to 68°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/\text{mmHg}) = [-0.2185 \times 6855.2/(T/K)] + 7.75768$; temp range –78.8 to 36.5°C (Antoine eq., Weast 1972–73)
70000 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.91429 - 1593.593/(289.355 + t/°C)$; temp range 0–30°C (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)
69440 (interpolated-Antoine eq., temp range 0–30°C, Dean 1985, 1992)
$\log (P/\text{mmHg}) = 7.771 - 1582.0/(288.0 + t/°C)$; temp range 0–30°C (Antoine eq., Dean 1985, 1992)

68700 (selected, Riddick et al. 1986)
$\log (P/\text{kPa}) = 5.3643 - 779.7/(196.5 + t/°\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
68800 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 5.54823 - 860.49/(-66.25 + T/\text{K})$; temp range 239–310 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = 115.1259 - 4.6278 \times 10^3/(T/\text{K}) - 42.197 \cdot \log (T/\text{K}) + 2.526 \times 10^{-2} \cdot (T/\text{K}) - 9.8906 \times 10^{-14} \cdot (T/\text{K})^2$; temp range 156–589 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

1652	(calculated-P/C, using Hine & Mookerjee 1975 data)
1248	(calculated-QSAR, Nirmalakhandan & Speece 1988)
1468	(computed value, Yaws et al. 1991)
1836	(γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

1.69	(calculated-π const., Hansch et al. 1968)
1.90	(shake flask, Log P Database, Hansch & Leo 1987)
1.90	(recommended, Sangster 1989)
1.90	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:
Hydrolysis: rate constant $k = 2.12 \times 10^7\ s^{-1}$ with $t_{1/2}$ = 38 d at 25°C and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:
Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (Darnall et al. 1976).
Surface water: $t_{1/2}$ = 38 d at 25°C and pH 7 based on hydrolysis rate constant (Mabey & Mill 1978)

TABLE 5.1.1.15.1
Reported aqueous solubilities and vapor pressures of 2-chloropropane at various temperatures

Aqueous solubility				Vapor pressure			
Rex 1906		Horvath 1982		Rex 1906		Stull 1947	
volumetric method		summary of literature data				summary of literature data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
0	440	0	4381	0	25558	−78.8	133.3
10	362	10	3607	10	38863	−61.1	666.6
20	305	20	3141	20	58062	−52.0	1333
30	304	25	2945	30	83953	−42.0	2666
		30	3031			−31.0	5333
						−23.5	7999
						−13.7	13332
						1.30	26664
						18.1	53329
						36.5	101325
						mp/°C	−117

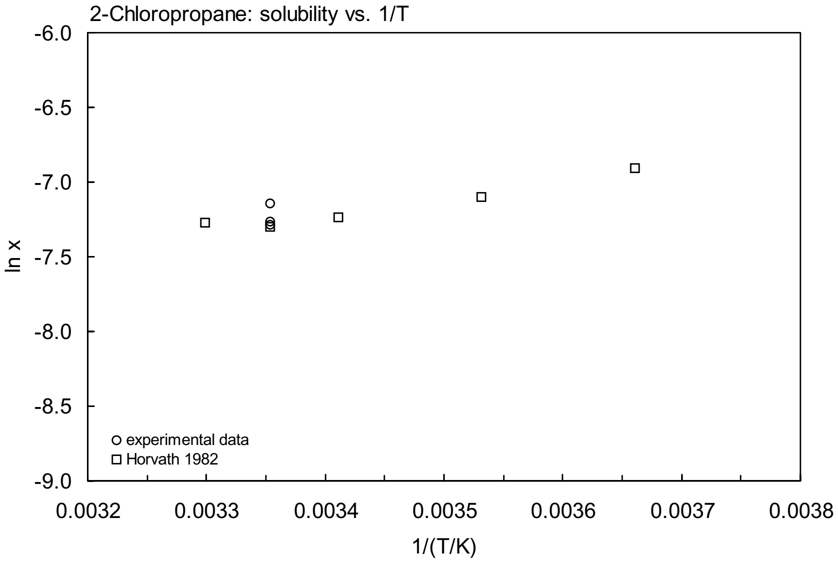


FIGURE 5.1.1.15.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-chloropropane.

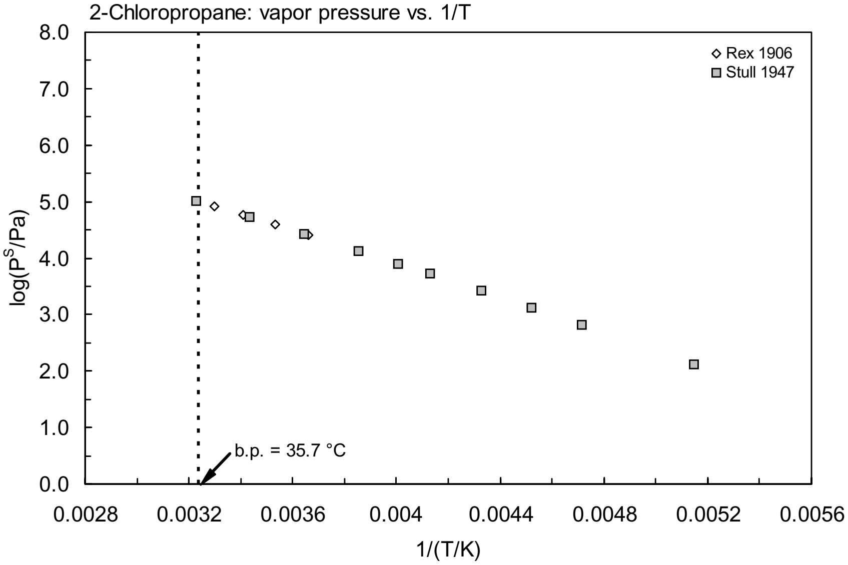
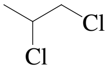


FIGURE 5.1.1.15.2 Logarithm of vapor pressure versus reciprocal temperature for 2-chloropropane.

5.1.1.16 1,2-Dichloropropane



Common Name: 1,2-Dichloropropane
Synonym: propylene chloride, propylene dichloride, α,β-propylene dichloride
Chemical Name: 1,2-dichloropropane
CAS Registry No: 78-87-5
Molecular Formula: 1,2-$C_3H_6Cl_2$, $CH_3CHClCH_2Cl$
Molecular Weight: 112.986
Melting Point (°C):
–100.53 (Lide 2003)
Boiling Point (°C):
96.40 (McGovern 1943; Timmermans 1950; Weast 1982–83; Dean 1985; Lide 2003)
Density (g/cm^3 at 20°C):
1.1560 (Dreisbach 1959, 1961; Horvath 1982; Weast 1982–83; Riddick et al. 1986)
1.1494 (25°C, Dreisbach 1959, 1961)
Molar Volume (cm^3/mol):
98 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)
115.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
36.33, 30.5 (25°C, normal bp, Dreisbach 1961)
36.40, 32.004 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
6.40 (calculated, Dreisbach 1959; quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
2800 (shake flask-interferometer, Gross 1929; Stephen & Stephen 1963)
2773 (Seidell 1940)
2700 (20°C, McGovern 1943)
2750 (measured by Dow Chemical, Dreisbach 1955–1961)
2096 (shake flask-GC, Jones et al. 1977/1978)
3520 (shake flask-GC, Chiou et al. 1979)
2800* (summary of literature data, Horvath 1982)
2420 (headspace-GC, McNally & Grob 1983)
2070 (30°C, headspace-GC, McNally & Grob 1984)
2600 (Dean 1985)
2740 (selected, Riddick et al. 1986; Howard 1990)
3000*, 2900 (20°C, 29.7°C, shake flask-GC/TC, measured range 0–90.4°C, Stephenson 1992)
3005, 3129, 3261 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
3287, 3706, 4152 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-UNIFAC, Tse et al. 1992)
2683, 2717, 3003 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
2650 (20°C, limiting activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
2740* (recommended, temp range 278.15–313.15 K, IUPAC-NIST Series, Horvath & Getzen 1999)
$S/(\text{wt\%}) = 3.3285 - 0.021464\cdot(T/K) + 3.7632 \times 10^{-5}\cdot(T/K)^2$, temp range 275–313 K (Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
7200* (isoteniscope method, measured range 15–99.7°C, Nelson & Young 1933)
$\log (P/\text{mmHg}) = 7.7085 - 1782.8/(T/K)$; temp range 15–100°C (isoteniscope, Nelson & Young 1933)
6930 (McGovern 1943)

6780* (Antoine eq. regression, temp range –7 to 141.6°C, Stull 1947)
16500* (44.78°C, ebulliometry, measured range 44.78–96.2°C, Dreisbach & Shrader 1949)
6620 (calculated-Antoine eq., Dreisbach 1959, 1961)
log (P/mmHg) = 6.96395 – 1295.9/(221.0 + t/°C); temp range 15–160°C (Antoine eq. for liquid state, Dreisbach 1959)
log (P/mmHg) = 6.96546 – 1296.4/(221.0 + t/°C); temp range 15–135°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = [–0.2185 × 8428.5/(T/K)] + 7.882416; temp range –38.5 to 96.8°C (Antoine eq., Weast 1972–73)
6720 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 6.98047 – 1308.138/(222.845 + t/°C); temp range 44.8–96.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
6720, 7120 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.10153 – 1305.689/(222.567 + t/°C), temp range 55.78–96.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
log (P/kPa) = 6.73547 – 1717.264/(266.9 + t/°C), temp range 15–99.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9807 – 1308.1/(222.8 + t/°C); temp range 45–96°C (Antoine eq., Dean 1985, 1992)
6622 (selected, Riddick et al. 1986)
log (P/kPa) = 6.08885 – 1295.9/(221.0 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
6620 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.08324 – 1292.64/(–52.52 + T/K); temp range 239–373 K (Antoine eq., Stephenson & Malanowski 1987)
5410, 8790, 13790 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 5.4819 – 2.1918 × 10^3/(T/K) + 2.6014·log (T/K) – 1.1751 × 10^{-2}·(T/K) + 7.3435 × 10^{-6}·$(T/K)^2$; temp range 173–572 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
298 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
31.21, 2261 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
280* (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)
ln (k_H/atm) = 19.60 – 4333/(T/K); temp range:1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
210 (calculated-P/C, Mackay & Yuen 1983)
286 (gas stripping-GC, Warner et al. 1987)
362* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 9.843 – 4708/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
233 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
150 (computed value, Yaws et al. 1991)
213, 324, 486 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
216, 347, 497 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
3.37, 5.93 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
222 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
226.8 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
232 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 4.878 – 1730/(T/K) (summary of literature data, Staudinger & Roberts 2001)
227.6* (EPICS-SPME, measured range 2–70°C, Görgényi et al. 2002)
ln K_{AW} = 9.49 – 3494.7/(T/K); temp range 2–70°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.00 (Hansch & Leo 1979)
1.98 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)
1.99* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

2.96 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

< 1.0 (fish, Kawasaki 1980; quoted, Howard 1990)
1.29 (calculated-K_{OW}, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

1.43 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
1.67 (silt loam soil, quoted from Chiou et al. 1979; Howard 1990)
1.70 (calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} < 50$ min in water from stirring in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975; quoted, Mills et al. 1982);
$t_{1/2} = 8$ min from a stirred solution 1.6 cm deep (Chiou et al. 1980; quoted, Howard 1990);
$t_{1/2} = 1.7$–10 d, estimated from an EXAMS model of the fate of 1,2-dichloropropane in a pond, river, and two lakes (Burns 1981; quoted, Howard 1990);
$t_{1/2} = 8.3$ h at 1 m depth of stirred aqueous solution (Lyman et al. 1982; quoted, Howard 1990);
$t_{1/2} \sim 5.5$ h for the removal from a stream of 1 m depth with 1 m/s current, based on laboratory-determined relative transfer coefficients (Cadena et al. 1984; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
photooxidation $t_{1/2} = 65$–646 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)
$k_{O3}(aq.) \leq 0.004\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with a half-life of 100 d at pH 7 (Yao & Haag 1991).

Hydrolysis: $k = 5.0 \times 10^{-6}\ h^{-1}$ at pH 7 to 9 and 25°C with a calculated $t_{1/2} = 15.8$ yr (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biodegradation: aerobic $t_{1/2}(aq.) = 4008$–30936 h, based on acclimated aerobic soil grab sample data (Roberts & Stoydin 1976; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}(aq.) = 16032$–123744 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4$–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
$t_{1/2} = 65$–646 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
$t_{1/2} > 23$ d, reaction with photochemically produced OH radical (Howard 1990).

Surface water: $t_{1/2} = 4008$–30936 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); measured rate constant $k \leq 0.004\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 100$ d at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 8016$–61872 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 4008$–30936 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.1.16.1
Reported aqueous solubilities of 1,2-dichloropropane at various temperatures

$$S/(wt\%) = 0.1300 + 1.43332 \times 10^{-2} \cdot (t/°C) - 4.99992 \times 10^{-4} \cdot (t/°C)^2 + 6.66654 \times 10^{-6} \cdot (t/°C)^3 \quad (1)$$

$$S/(wt\%) = 3.3285 - 0.021464 \cdot (T/K) + 3.7632 \times 10^{-5} \cdot (T/K)^2 \quad (2)$$

Horvath 1982		Stephenson 1992		Tse et al. 1992		Horvath & Getzen 1999	
summary of literature data		shake flask-GC		activity coefficient		recommended IUPAC-NIST	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
10	2300	0	2900	20	3005	5	2799
20	2700	9.5	2800	30	3129	10	2680
25	2800	20	3000	40	3261	15	268-
30	2900	29.7	2900			20	2700
		40.3	3000			25	2740
eq.1	S/wt%	49.8	3200	**Wright et al. 1992**		30	2800
		60	3500	**activity coefficient**		35	2880
		70.5	3900	**t/°C**	**S/g·m^{-3}**	40	2970
		80.2	4700				
		90.4		20	2583	eq. 2	S/wt%
				30	2717	temp range 275–313 K	
				40	3003		

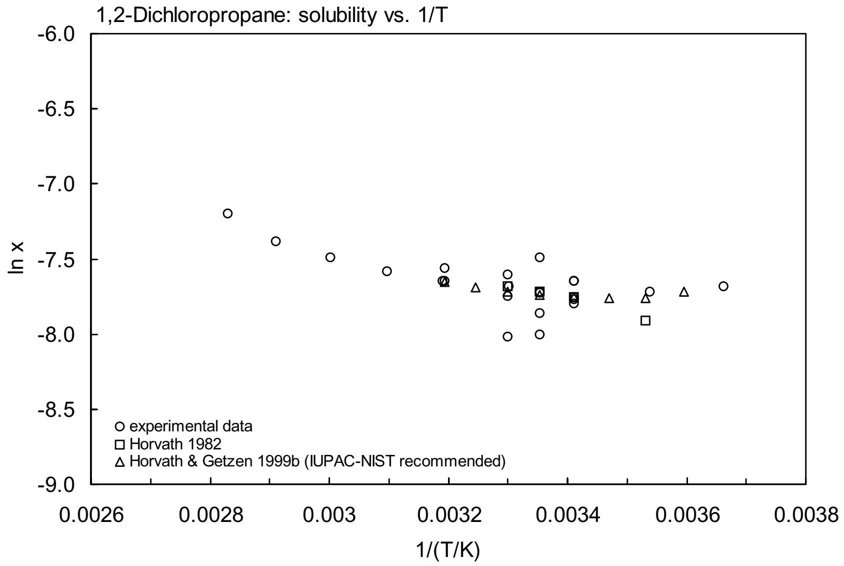


FIGURE 5.1.1.16.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.16.2
Reported vapor pressures of 1,2-dichloropropane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Nelson & Young 1933		Stull 1947		Dreisbach & Shrader 1949	
static method		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
15.0	4400	–7.0	133.3	44.78	16500
20.0	5600	17.3	666.6	69.0	42066
25.0	7199	29.4	1333	83.18	67661
30.0	8999	42.3	2666	96.2	101325
35.0	11199	57.2	5333		
40.0	13799	66.4	7999		
45.0	16839	75.7	13332		
50.0	20625	97.8	26664		
55.0	24065	118.5	53329		
60.0	30317	141.6	101325		
65.0	36397				
70.0	43570	mp/°C	–34.4		
75.0	51729				
80.0	61235				
85.0	71874				
90.0	84059				
95.0	97792				
96.0	100525				
96.4	101325				
99.7	112937				

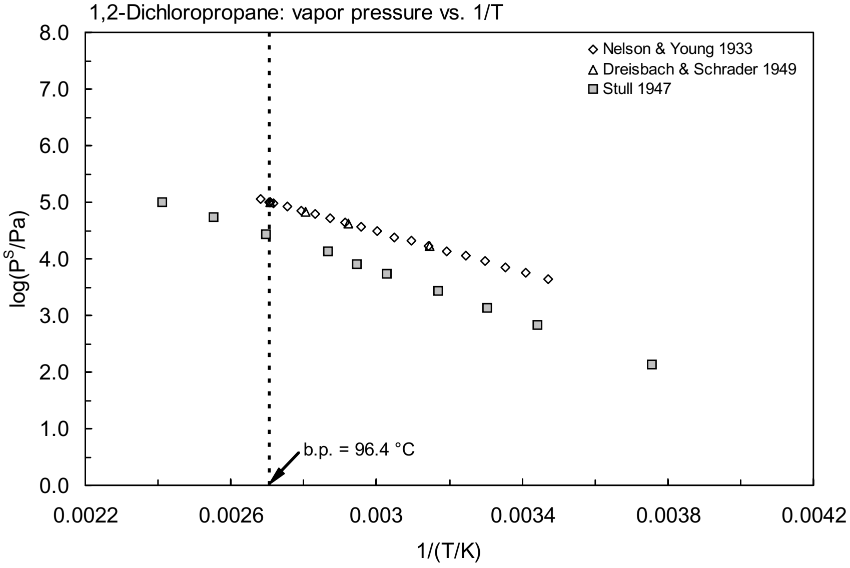


FIGURE 5.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichloropropane.

TABLE 5.1.1.16.3

Reported Henry's law constants of 1,2-dichloropropane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm·m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Leighton & Calo 1981		**Ashworth et al. 1988**		**Tse et al. 1992**		**Görgényi et al. 2002**	
equilibrium cell-GC		**EPICS-GC**		**activity coefficient**		**EPICS-SPME method**	
t/°C	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**
1.90	83.5	10	123.6	20	213	2	82.35
13.5	164.5	15	127.7	30	324	6	109
15.7	185.3	20	192.5	40	486	10	134.2
17.1	239.7	25	361.7			18	203.3
22.0	239.7	30	289.8			25	227.6
24.9	280.0			**Wright et al. 1992**		30	341.8
		eq. 4	H/(atm m³/mol)	**activity coefficient**		40	524.9
eq. 3	k_H/atm	A	9.843	**t/°C**	**H/(Pa m³/mol)**	50	759.8
A	19.6	B	4708			60	1014
B	4333			20	216	70	1226
				35	347		
				50	497	eq. 1	K_{AW}
						A	9.49
						B	3494.7

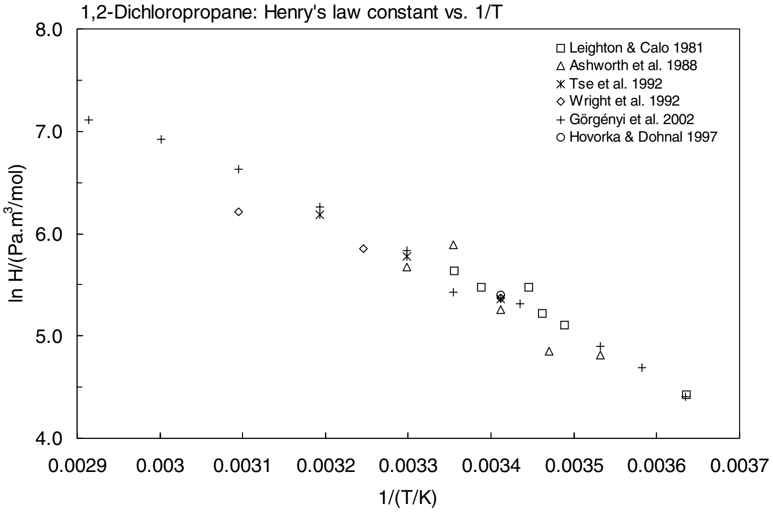


FIGURE 5.1.1.16.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dichloropropane.

TABLE 5.1.1.16.4
Reported octanol-water partition coefficient of 1,2-dichloropropane at various temperatures

Bhatia & Sandler 1995	
relative GC-RT technique	
t/°C	log K_{OW}
25	1.99
35	1.99
50	1.99
enthalpy of transfer	
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$	
log $K_{OW} = A - \Delta H/2.303RT$	
A	1.0195
ΔH	–20.2

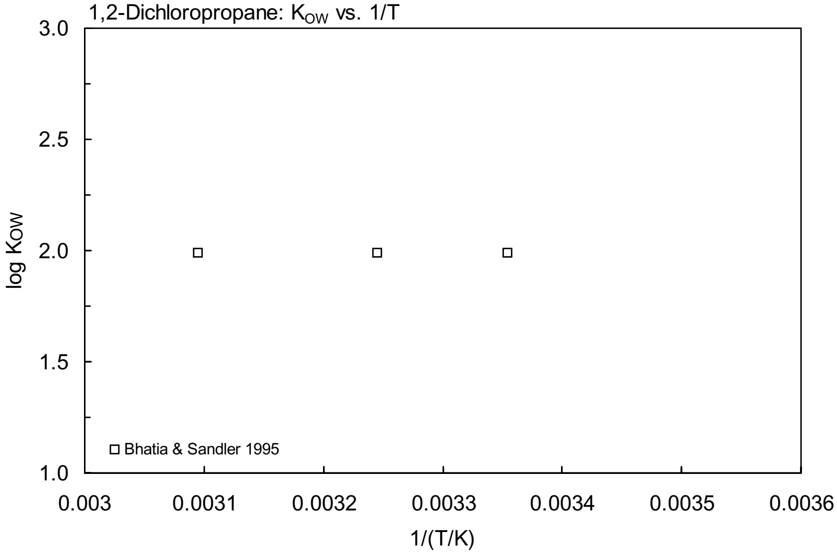
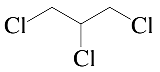


FIGURE 5.1.1.16.4 Logarithm of K_{OW} versus reciprocal temperature for 1,2-dichloropropane.

5.1.1.17 1,2,3-Trichloropropane



Common Name: 1,2,3-Trichloropropane
Synonym:
Chemical Name: 1,2,3-trichloropropane
CAS Registry No: 96-18-4
Molecular Formula: 1,2,3-$C_3H_5Cl_3$, $CH_2ClCHClCH_2Cl$
Molecular Weight: 147.431
Melting Point (°C):
–14.7 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
157 (Lide 2003)
Density (g/cm^3 at 20°C):
1.3888 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
1.3832 (25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm^3/mol):
136.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
46.93, 37.12 (25°C, normal bp, Dreisbach 1961; Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1900 (20°C, literature average, Dilling 1977)
1896 (recommended, Horvath 1982)
1900 (selected, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
492 (extrapolated-Antoine eq., Dreisbach 1961)
$\log (P/mmHg) = 6.98716 - 1502.3/(209.0 + t/°C)$; temp range 64–204°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = [-0.2185 \times 10714.3/(T/K)] + 8.326893$; temp range 9.0–158°C (Antoine eq., Weast 1972–73)
266.6, 533.2 (20°C, 30°C, Verschueren 1983)
492.0 (calculated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.11206 - 1502.3/(-64.15 + T/K)$; temp range 337–477 K (Antoine eq., Stephenson & Malanowski 1987)
413, 960 (quoted, calculated-solvatochromic parameters. and UNIFAC, Banerjee et al. 1990)
$\log (P/mmHg) = -3.9501 - 2.4501 \times 10^3/(T/K) + 6.6887 \cdot \log (T/K) - 1.4991 \times 10^{-2} \cdot (T/K) + 7.3403 \times 10^{-6} \cdot (T/K)^2$; temp range 258–652 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
32.22 (calculated-C_A/C_W, Dilling 1977)
36.1* (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)
$\ln (k_H/atm) = 14.61 - 3477/(T/K)$; temp range:1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
24.91* (25.6°C, EPICS-GC, tap water, measured range 25.6–45°C, Tancréde & Yanagisawa 1990)
$\log K_{AW} = 3.351 - 1606/(T/K)$; temp range 26.5–45°C (EPICS measurements, Tancréde & Yanagisawa 1990)
34.4 (computed value, Yaws et al. 1991)
22.31 (interpolated from Tancréde & Yanagisawa 1990, Tancréde et al. 1992)

23.71 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
22.74 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 3.073 – 1496/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

2.63 (estimated, Abernethy et al. 1988)
1.98 (quoted, Van Leeuwen et al. 1992; Verhaar et al. 1992)
2.25, 2.36 (quoted, calculated-molar volume, Wang et al. 1992)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.98; 1.89; 1.92 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43, batch equilibrium-sorption isotherm, Walton et al. 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization: evaporation $t_{½}$ = 51 min from dilute aqueous solution (Dilling 1975)
Evaporation $t_{½}$(exptl) = 56.1 min, $t_{½}$(calc) = : 18 min, 44.7 min from water (Dilling 1977)
Photolysis:
Oxidation: photooxidation $t_{½}$ = 61–613 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: k = 1.8×10^{-6} h^{-1} at pH 7 to 9 at 25°C with a calculated $t_{½}$ = 44 yr (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).
Biodegradation: aerobic $t_{½}$(aq.) = 4320–8640 h, based on acclimated aerobic grab sample test data for 1,3-dichloropropane (Roberts & Stoydin 1976; quoted, Howard et al. 1991); anaerobic $t_{½}$(aq.) = 17280–34560 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
$t_{½}$ = 61–613 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: $t_{½}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Ground water: $t_{½}$ = 8640–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: disappearance $t_{½}$ = 2.7 d was calculated from first-order kinetic for volatilization loss of mixtures in soils (Anderson et al. 1991);
$t_{½}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biota:

TABLE 5.1.1.17.1
Reported Henry's law constants of 1,2,3-trichloropropane at various temperatures

Leighton & Calo 1981	
equilibrium cell-GC	
t/°C	H/(Pa m^3/mol)
1.90	21.27
13.5	20.90
15.7	24.71
17.1	25.86
22.0	27.58
24.9	36.13
ln (k_H/atm) = A – B/(T/K)	
A	14.61
B	3477

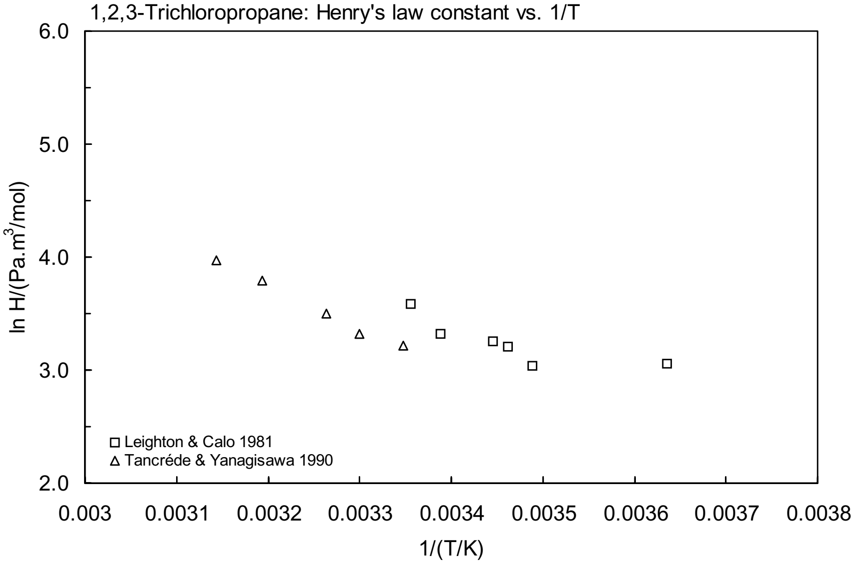
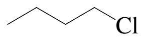


FIGURE 5.1.1.17.1 Logarithm of Henry's law constant versus reciprocal temperature for 1,2,3-trichloropropane.

5.1.1.18 1-Chlorobutane (*n*-Butyl chloride)



Common Name: 1-Chlorobutane
Synonym: *n*-butyl chloride, butyl chloride
Chemical Name: 1-chlorobutane, *n*-butyl chloride
CAS Registry No: 109-69-3
Molecular Formula: C_4H_9Cl, $CH_3CH_2CH_2CH_2Cl$
Molecular Weight: 92.567
Melting Point (°C):
–123.1 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
78.44 (Dreisbach 1959, 1961; Horvath 1982; Dean 1985)
78.4 (Lide 2003)
Density (g/cm^3 at 20°C):
0.8862, 0.8808 (20°C, 25°C, Dreisbach 1959, 1961; Horvath 1982)
0.8857, 0.8810 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
117.1 (calculated-Le Bas method at normal boiling point)
104.5 (20°C, calculated-density)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
30.02, 33.32 (normal bp, 25°C, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
666 (12.5°C, shake flask, Fühner 1924)
640 (Seidell 1940)
741 (Kakovsky 1957)
667 (17.5°C, Saracco & Spaccamela Marchetti 1958)
671 (20°C, exptl., Korenman et al. 1971; Horvath 1982)
614.7* (summary of literature data, Horvath 1982)
872 (generator column-HPLC, Tewari et al. 1982)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
4173* (20°C, static method-manometer, measured range 20–70°C, Smyth & Engel 1929)
14170* (interpolated compiled data, temp range –49 to 77.8°C, Stull 1947)
13650 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.93790 – 1227.43/(224.1 + t/°C); temp range 0–123°C (Antoine eq. for liquid state, Dreisbach 1959)
log (P/mmHg) = 6.93790 – 1227.433/(224.1 + t/°C); temp range 1–116°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.93790 – 1227.433/(224.10 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
10639* (19.7°C, differential thermal analysis, measured range –16.7 to 78.5 °C, Kemme & Kreps 1969)
log (P/mmHg) = [–0.2185 × 8144.8/(T/K)] + 7.979366; temp range –49 to 77.8°C (Antoine eq., Weast 1972–73)
14719* (26.85°C, differential thermal analysis, measured range 26.85–80.0°C, Gutsche & Knapp 1982)
log (P/mmHg) = 6.83694 – 1173.79/(218.13 + t/°C), temp range: –17 to 78.6°C (Antoine eq., Dean 1985, 1992)
13300 (24.47°C, selected, Riddick et al. 1986)
log (P/kPa) = 6.0514 – 1216.82/(222.33 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
13660 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.0628 - 1227.433/(-49.05 + T/K)$; temp range 257–389 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = 35.7808 - 2.8632 \times 10^3/(T/K) - 8.8957 \cdot \log (T/K) + 5.1598 \times 10^{-11} \cdot (T/K) + 3.5488 \times 10^{-6} \cdot (T/K)^2$; temp range 150–537 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1970	(exptl-$1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975)
1800, 8600	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1530*	(23°C, equilibrium cell-concn ratio-GC/FID, measured range 1–23°C, Leighton & Calo 1981)

$\ln (k_H/atm) = 18.51 - 3482/(T/K)$; temp range1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

1708	(computed value, Yaws et al. 1991)
1878	(γ^∞ from gas stripping-GC, Li et al. 1993)
1485	(20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
1384	(20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.488 - 1388/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.39	(shake flask-GC, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)
2.64	(shake flask, Hansch & Leo 1979; 1987)
2.55	(generator column-GC, DeVoe et al. 1981)
2.55	(generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)
2.64	(recommended, Sangster 1989, 1993)
2.64	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.72	(head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 5.1.1.18.1
Reported aqueous solubilities and Henry's law constants of 1-chlorobutane at various temperatures

$$S/(wt\%) = 0.07703 - 6.75497 \times 10^{-4} \cdot (t/°C) - 1.00170 \times 10^{-10} \cdot (t/°C)^2 + 8.50030 \times 10^{-8} \cdot (t/°C)^3 \qquad (1)$$

Aqueous solubility		Henry's law constant	
Horvath 1982		Leighton & Calo 1981	
summary of literature data		equilibrium cell-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)
0	770.3	1.0	593.7
10	703.6	3.0	684.5
20	642.0	12.4	979.2
25	614.7	12.5	1038
30	590.6	17.9	1265

TABLE 5.1.1.18.1 (*Continued*)

Aqueous solubility		Henry's law constant	
Horvath 1982		Leighton & Calo 1981	
summary of literature data		equilibrium cell-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)
		22.7	1251
eq. 1	S/wt%	23.0	1530
		ln (k_H/atm) = A – B/(T/K)	
		A	18.51
		B	3482

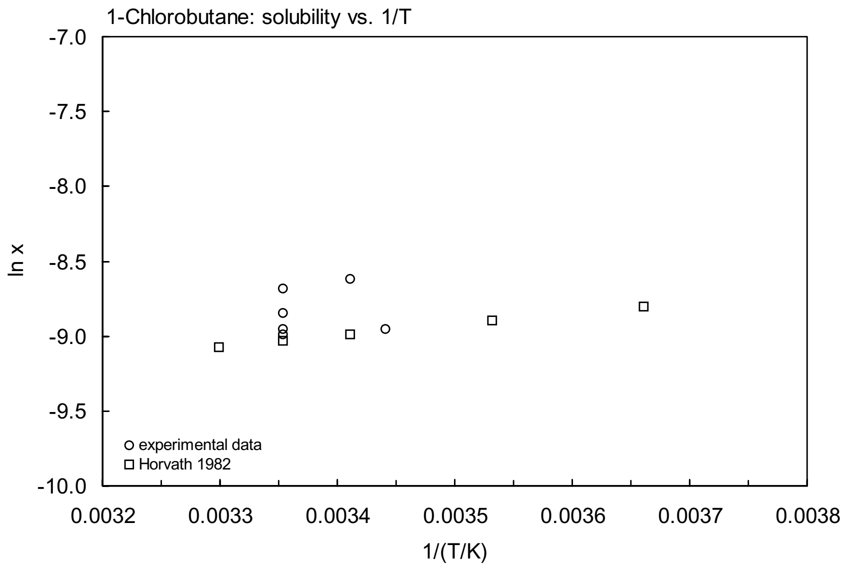


FIGURE 5.1.1.18.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1-chlorobutane.

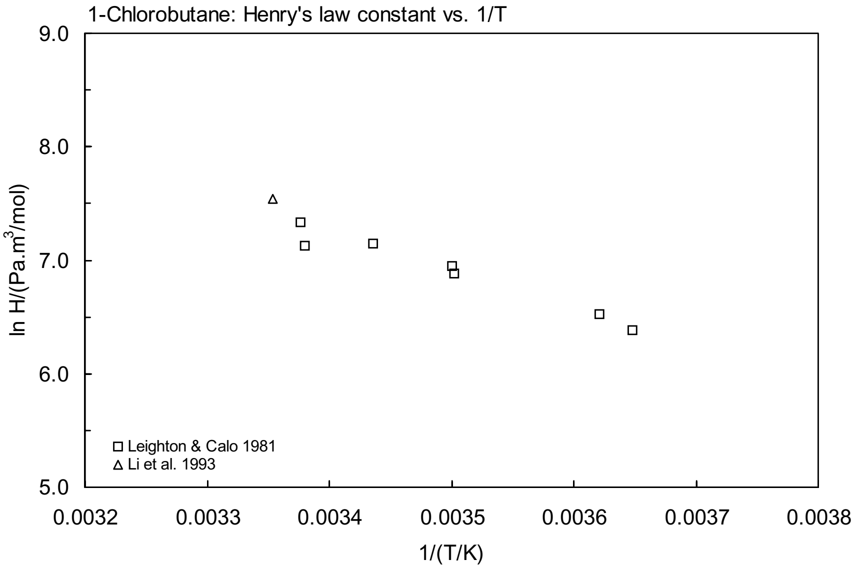


FIGURE 5.1.1.18.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chlorobutane.

TABLE 5.1.1.18.2
Reported vapor pressures of 1-chlorobutane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log(T/K)$	(4)		

Smyth & Engel 1929		**Stull 1947**		**Kemme & Kreps 1969**		**Gutsche & Knapp 1982**	
static-manometry		**summary of literature data**		**static method-DTA***		**Vapor-liquid equilibrium**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
20.0	4173	–49.0	133.3	–16.7	1347	26.85	14719
30.0	6799	–28.9	666.6	–10.5	2026	30.0	17001
40.0	10959	–18.6	1333	–6.20	2640	50.0	38434
50.0	16892	–7.40	2666	0.80	3946	51.85	41397
60.0	25278	5.0	5333	6.20	5360	78.85	96925
70.0	36170	13.0	7999	12.0	7306	80.0	106255
		24.0	13332	19.7	10639		
		40.0	26664	28.8	16212		
		55.8	53329	41.1	27078		
		77.8	101325	51.3	40263		
				65.5	66541		
		mp/°C	–123.1	78.5	101165		
				eq. 2	P/mmHg		
				A	6.87098		
				B	1182.903		
				C	218.285		

*DTA—differential thermal analyzer

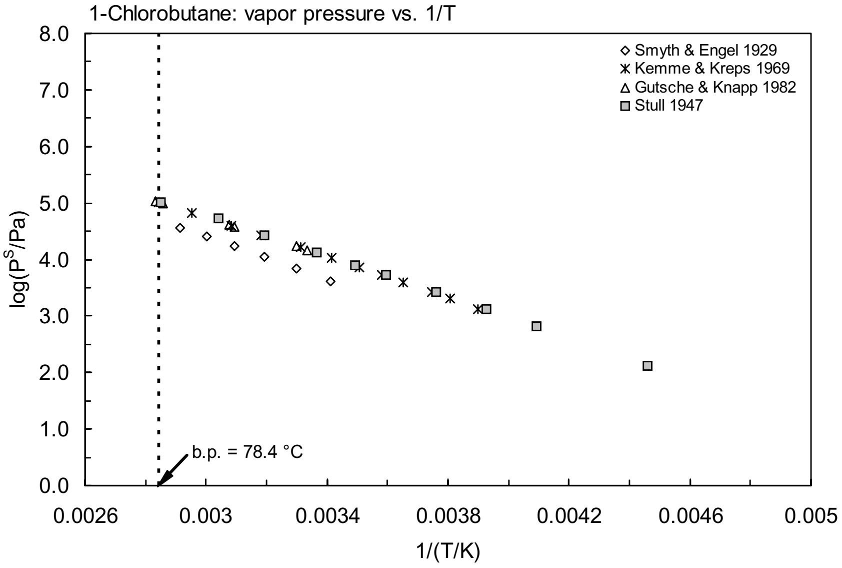
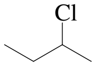


FIGURE 5.1.1.18.3 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorobutane.

5.1.1.19 2-Chlorobutane



Common Name: 2-Chlorobutane
Synonym: methylethylchloromethane, *sec*-butyl chloride
Chemical Name: 2-chlorobutane, methylethylchloromethane, *sec*-butyl chloride
CAS Registry No: 78-86-4
Molecular Formula: C_4H_9Cl, $CH_3CH_2CHClCH_3$
Molecular Weight: 92.567
Melting Point (°C):
 –131.3 (Dreisbach 1961; Horvath 1982; Lide 2003)
 –113.3, –140.5 (racemic, active, Riddick et al. 1986)
Boiling Point (°C):
 68.25 (Dreisbach 1961; Horvath 1982; Riddick et al. 1986)
 68.2 (Lide 2003)
Density (g/cm^3 at 20°C):
 0.8732, 0.8677 (20°C, 25°C, Dreisbach 1961; Horvath 1982; Dean 1985)
 0.8732 (racemic, Riddick et al. 1986)
Molar Volume (cm^3/mol):
 117.1 (calculated-Le Bas method at normal boiling point)
 106.0 (20°C, calculated-density)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 31.81, 29.20 (25°C, bp, Dreisbach 1961)
 31.56, 29.20 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
 1000 (volumetric method, Wright & Schaffer 1932)
 1000 (Dean 1985; Riddick et al. 1986)
 1070, 930, 850, 820, 840, 920 (0, 5, 10, 15, 20, 35°C, tentative values, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)
 $S/(wt\%) = 8.9653 - 0.061598\cdot(T/K) + 1.0678 \times 10^{-4}\cdot(T/K)^2$, temp range 273–298 K (equation derived from reported solubility data, Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 20210 (interpolated-Antoine eq., Dreisbach 1961)
 $\log (P/mmHg) = 6.94469 - 1195.8/(226.0 + t/°C)$; temp range –7 to 104°C (Antoine eq. for liquid state, Dreisbach 1961)
 $\log (P/mmHg) = [-0.2185 \times 7407.9/(T/K)] + 7.625620$; temp range –60.2 to 68°C (Antoine eq., Weast 1972–73)
 $\log (P/mmHg) = 6.79923 - 1149.12/(224.68 + t/°C)$; temp range 0–40°C (Antoine eq., Dean 1985, 1992)
 $\log (P/kPa) = 6.1222 - 1145.2/(234.4 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
 20200 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/kPa) = 6.06958 - 1195.8/(-47.15 + T/K)$; temp range 266–377 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/mmHg) = 28.2992 - 2.4355 \times 10^3/(T/K) - 7.359\cdot\log (T/K) - 1.3048 \times 10^{-11}\cdot(T/K) + 3.0834 \times 10^{-6}\cdot(T/K)^2$; temp range 142–521 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 2268* (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)
 $\ln (k_H/atm) = 22.29 - 4499/(T/K)$; temp range1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

1869	(computed value, Yaws et al. 1991)
1886	(20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.129 - 1829/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

1.51	(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

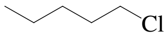
Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radicals (Darnall et al. 1976).

TABLE 5.1.1.19.1
Reported Henry's law constants of 2-chlorobutane at various temperatures

Leighton & Calo 1981	
equilibrium cell-GC	
t/°C	**H/(Pa m³/mol)**
1.90	653.3
13.5	1411
15.7	1545
17.1	1625
22.0	2023
24.9	2268
$\ln(k_H/\text{atm}) = A - B/(T/K)$	
A	22.29
B	4499

5.1.1.20 1-Chloropentane (*n*-Amyl chloride)



Common Name: 1-Chloropentane
Synonym: *n*-amyl chloride, monochloropentane, pentyl chloride
Chemical Name: *n*-amyl chloride, 1-chloropentane, pentyl chloride
CAS Registry No: 543-59-9
Molecular Formula: $C_5H_{11}Cl$, $CH_3CH_2CH_2CH_2CH_2Cl$
Molecular Weight: 106.594
Melting Point (°C):
–99.0 (Dreisbach 1961; Horvath 1982; Riddick et al. 1982; Dean 1985; Lide 2003)
Boiling Point (°C):
108.4 (Lide 2003)
Density (g/cm^3 at 20°C):
0.8818 (20°C, Weast 198–83; Horvath 1982)
0.8820, 0.8770 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
120.9 (20°C, calculated-density)
139.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
38.24, 32.77 (25°C, bp, Dreisbach 1961; Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
200 (volumetric method, Wright & Schaffer 1932)
789 (shake flask-residue volume method, Booth & Everson 1948)
190.6* (24.3°C, converted-distribution coeff., temp range 2.5–26.1°C, Leighton & Calo 1981)
198.2* (summary of literature data, Horvath 1982)
200 (Dean 1985; Riddick et al. 1986)
201* (tentative values, measured range 5–35°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)
$S/(\mathrm{wt\%}) = 0.55726 - 3.7269 \times 10^{-3}\cdot(T/K) + 6.457 \times 10^{-6}\cdot(T/K)^2$, temp range 276–310 K (equation derived from reported solubility data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4142 (calculated-Antoine eq, Dreisbach 1961)
$\log (P/\mathrm{mmHg}) = 6.96617 - 1332.890/(218.5 + t/°C)$; temp range 24–148°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/\mathrm{mmHg}) = 6.96617 - 1332.890/(218.50 + t/°C)$; pressure range 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
4142 (selected, Riddick et al. 1986)
$\log (P/\mathrm{kPa}) = 5.93641 - 1271.15/(215.0 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
4148 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/\mathrm{kPa}) = 6.09107 - 1332.89/(T/K - 54.65)$; temp range 289–409 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/\mathrm{mmHg}) = -4.4886 - 2.2604 \times 10^3/(T/K) + 7.8088\cdot\log (T/K) - 2.3675 \times 10^{-2}\cdot(T/K) + 1.4884 \times 10^{-5}\cdot(T/K)^2$; temp range 174–568 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2209	(exptl.- $1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975)
2480, 13010	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
2376*	(24.3°C, equilibrium cell-concn ratio-GC/FID, measured range 2.5–26.1°C, Leighton & Calo 1981)

$\ln (k_H/\text{atm}) = 23.04 - 4727/(T/K)$; temp range 2.5–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

4942	(computed value, Yaws et al. 1991)
2407	(activity coefficient γ^∞ from gas stripping-GC, Li et al. 1993)
1835	(20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.455 - 1928/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

2.41	(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 5.1.1.20.1
Reported aqueous solubilities and Henry's law constant of 1-chloropentane at various temperatures

$$S/(\text{wt}\%) = 0.02426 - 1.79166 \times 10^{-4}\cdot(t/°C) + 1.49999 \times 10^{-7}\cdot(t/°C)^2 - 3.33355 \times 10^{-9}\cdot(t/°C)^3 \quad (1)$$

$$S/(\text{wt}\%) = 0.55726 - 3.7269 \times 10^{-3}\cdot(T/K) + 6.457 \times 10^{-6}\cdot(T/K)^2 \quad (2)$$

Aqueous solubility						**Henry's law constant**	
Leighton & Calo 1981		**Horvath 1982**		**Horvath & Getzen 1999b**		**Leighton & Calo 1981**	
converted-distribution coeff.		**summary of literature data**		**summary of literature data**		**equilibrium cell-GC**	
t/°C	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**t/°C**	**H/(Pa m^3/mol)**
2.5	200.6	0	242.6	5	202	2.5	661
7.0	205.2	10	224.8	10	197	7.0	846.6
12.9	196.8	20	207.1	15	195	12.9	1246
18.0	195.0	25	198.2	20	196	18.0	1654
19.5	200.5	30	189.3	25	210	19.5	1742
24.3	190.6			30	209	24.3	2376
26.1	203.2	eq. 1	S/wt%	35	220	26.1	2404
				eq. 2	S/wt%	ln k_H/atm = A –B/(T/K)	
				temp range 276–310 K		A	23.04
						B	4727

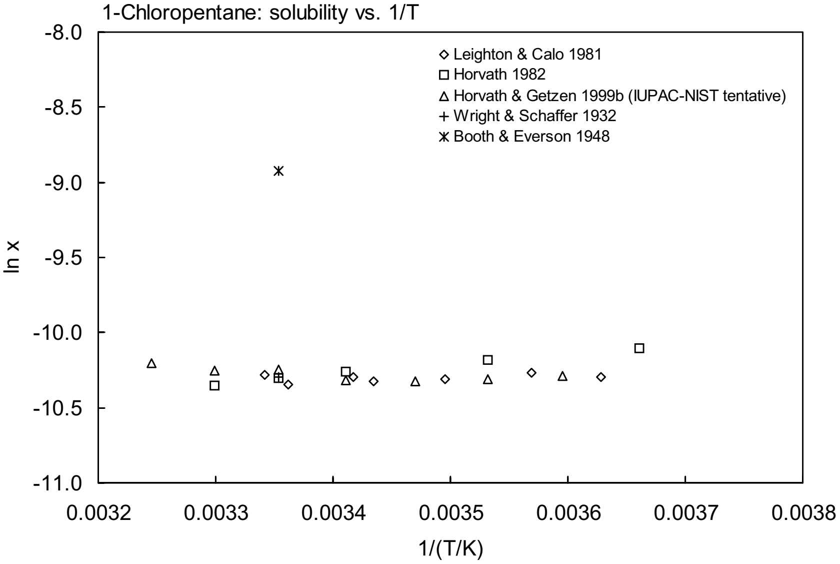


FIGURE 5.1.1.20.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1-chloropentane.

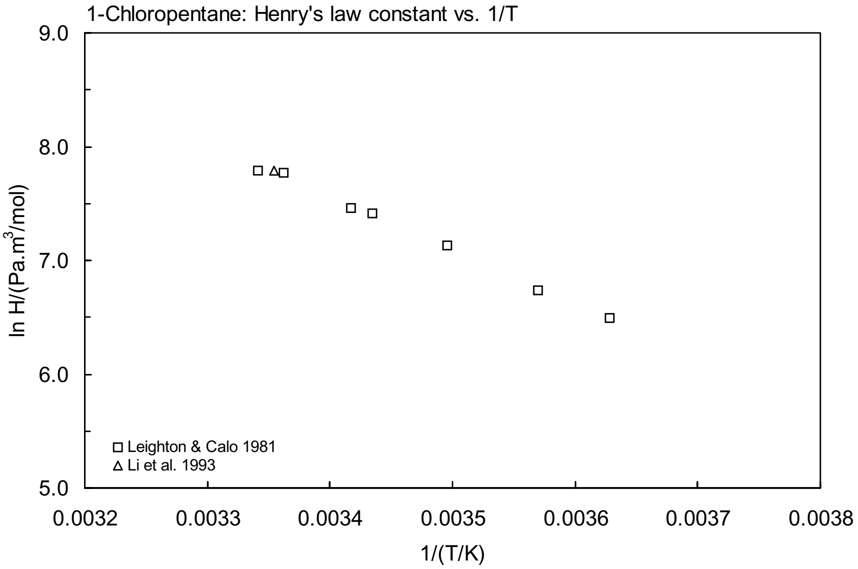
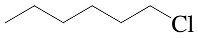


FIGURE 5.1.1.20.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chloropentane.

5.1.1.21 1-Chlorohexane



Common Name: 1-Chlorohexane
Synonym: *n*-hexyl chloride
Chemical Name: 1-chlorohexane
CAS Registry No: 544-10-5
Molecular Formula: $C_6H_{13}Cl$
Molecular Weight: 120.620
Melting Point (°C):
–94 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
135.1 (Lide 2003)
Density (g/cm^3):
0.8785; 0.8739 (20°C, 25°C, Dreisbach 1961)
0.8785 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
137.7 (20°C, calculated-density, Stephenson & Malanowski 1987)
161.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
43.22, 35.39 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
83.6 (volumetric method, Wright & Schaffer 1932)
57.93* (23.0°C, converted-distribution coeff., temp range 1.0–23.0°C, Leighton & Calo 1981)
91.01* (summary of literature data, Horvath 1982)
54.3* (tentative values, measured range 5–25°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)
S/(wt%) = $-0.019959 + 8.852 \times 10^{-5} \cdot (T/K)$, temp range 274–296 K (equation derived from reported solubility data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1284 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 7.0115 – 1437.05/(213.4 + t/°C); temp range 46–178°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 7.0115 – 1437.05/(213.4 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
1387* (26.7°C, differential thermal analysis, measured range 15–135.6°C, Kemme & Kreps 1969)
log (P/mmHg) = 6.76886 – 1304.968/(t/°C + 200.058); temp range 15–135.6°C (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)
1230 (interpolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.05136 – 1461.72/(t/°C + 136.92); temp range 15–136°C (Antoine eq. based on exptl. data of Kemme & Keeps 1969, Boublik et al. 1973)
1246 (interpolated, Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.89376 – 1304.968/(T/K – 73.092); temp range: 288–409 K (Antoine eq., Stephenson & Malanowski 1987)
1260 (interpolated-Antoine eq., Dean 1992)
log (P/mmHg) = 7.05136 – 1461.72/(t/°C + 215.57); temp range 15–136°C (Antoine eq., Dean 1992)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2312* (23°C, equilibrium cell-concn ratio-GC/FID, measured range 1–23°C, Leighton & Calo 1981)
$\ln(k_H/\text{atm}) = 22.16 - 4469/(T/K)$; temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
1899 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 6.073 - 1812/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

3.68 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 5.1.1.21.1
Reported aqueous solubilities and Henry's law constant of 1-chlorohexane at various temperatures

$$S/(\text{wt\%}) = 0.01172 - 0.000313(t/°C) - 1.078 \times 10^{-5}\cdot(t/°C)^2 - 4.58 \times 10^{-7}\cdot(t/°C)^3 \quad (1)$$
$$S/(\text{wt\%}) = -0.019959 + 8.852 \times 10^{-5}\cdot(T/K) \quad (2)$$

Aqueous solubility						**Henry's law constant**	
Leighton & Calo 1981		**Horvath 1982**		**Horvath & Getzen 1999b**		**Leighton & Calo 1981**	
converted-distribution coeff.		**summary of literature data**		**summary of literature data**		**equilibrium cell-GC**	
t/°C	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**t/°C**	**H/(Pa m^3/mol)**
1.0	36.87	0	117.2	5	46.7	1.0	728.6
3.0	49.46	10	101.1	10	51.1	3.0	666.6
12.4	56.45	20	97.08	15	55.5	12.4	1219
12.5	52.48	25	91.01	20	59.9	12.5	1328
17.9	61.87	30	77.66	25	64.3	17.9	1593
19.1	59.29			30	209	22.7	2118
22.7	62.37	eq. 1	S/wt%	35	220	23.0	2312
23.0	57.93						
				eq. 2	S/wt%	$\ln k_H/\text{atm} = A - B/(T/K)$	
				temp range 274–296 K		A	22.16
						B	4459

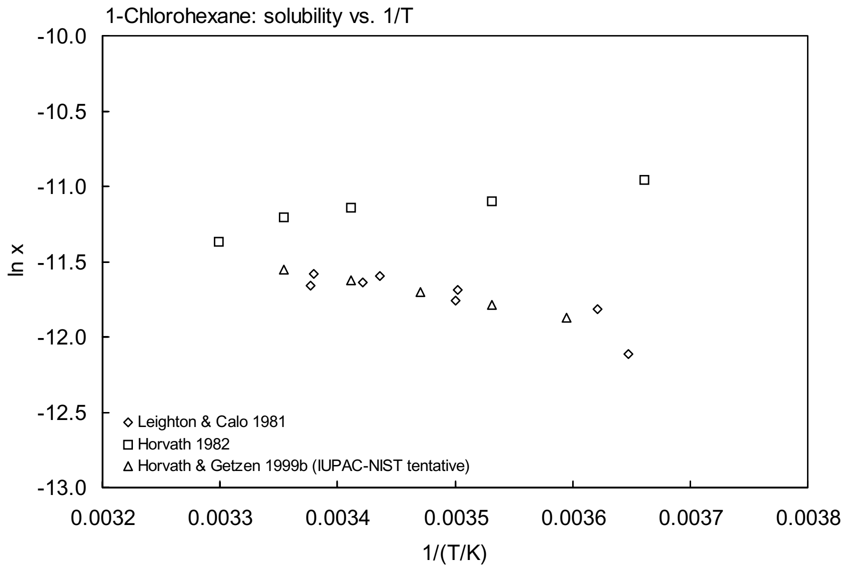


FIGURE 5.1.1.21.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1-chlorohexane.

TABLE 5.1.1.21.2
Reported vapor pressures of 1-chlorohexane at various temperatures

Kemme & Kreps 1969			
Static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
15.0	667	104.6	40757
26.7	1387	120.3	66781
33.1	2000	135.6	103191
38.6	2680		
46.7	4013	log P = A − B/(C + t/°C)	
52.6	5320		P/mmHg
59.7	7333	A	6.76886
68.4	10639	B	1304.968
79.5	16745	C	200.058
92.6	27091		

*DTA—differential thermal analyzer

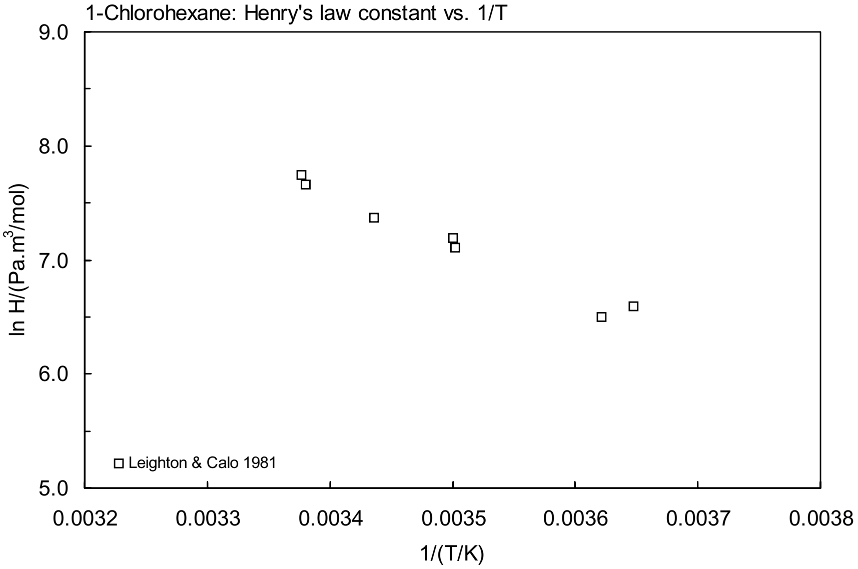


FIGURE 5.1.1.21.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chlorohexane.

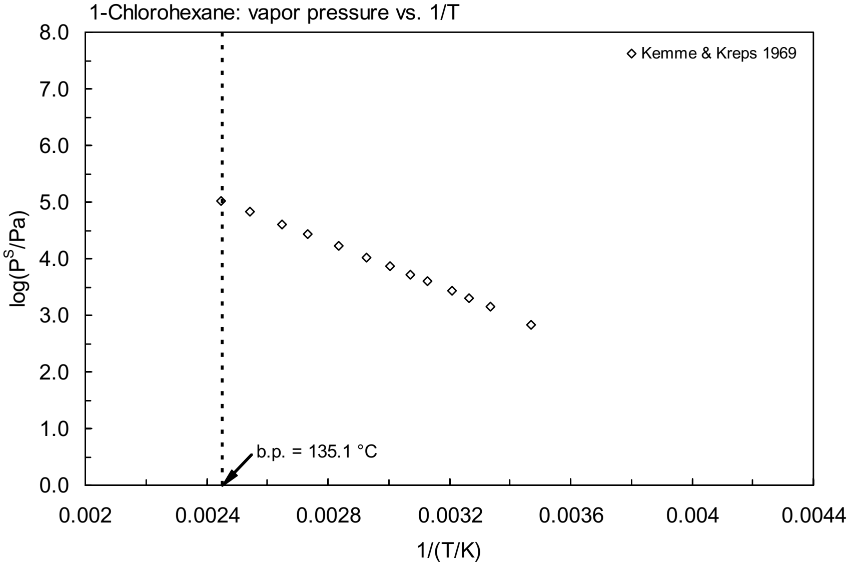
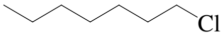


FIGURE 5.1.1.21.3 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorohexane.

5.1.1.22 1-Chloroheptane



Common Name: 1-Chloroheptane
Synonym: heptyl chloride
Chemical Name: 1-chloroheptane
CAS Registry No: 629-06-1
Molecular Formula: $C_7H_{15}Cl$
Molecular Weight: 134.647
Melting Point (°C):
–69.5 (Dreisbach 1961; Weast 1982–83; Lide 2003)
Boiling Point (°C):
160.4 (Lide 2003)
Density (g/cm^3):
0.8758, 0.8715 (20°C, 25°C, Dreisbach 1961)
0.8758 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
153.7 (20°C, calculated-density, Stephenson & Malanowski 1987)
183.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
48.19, 37.95 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
13.6 (generator column-GC/FID, Tewari et al. 1982; Miller et al. 1985)
13.6 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
404 (calculated-Antoine eq., Dreisbach 1961)
$\log (P/mmHg) = 7.0650 - 1539.35/(208.8 + t/°C)$; temp range 67–206°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = 7.0650 - 1539.35/(208.8 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
680* (34.4°C, differential thermal analysis, measured range 34.4–160°C, Kemme & Kreps 1969)
$\log (P/mmHg) = 6.83820 - 1410.064/(t/°C + 195.639)$; temp range 34.4–160.1°C (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)
336.6 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 6.05057 - 1459.652/(t/°C + 160.428)$; temp range 34.4–160°C (Antoine eq. based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)
$\log (P_L/kPa) = 6.9631 - 1410.064/(T/K - 77.511)$; temp range 307–434 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = 6.91670 - 1453.96/(t/°C + 199.83)$; temp range 36–160°C (Antoine eq., Dean 1992)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{OW}$:
4.08 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

TABLE 5.1.1.22.1
Reported vapor pressures of 1-chloroheptane at various temperatures

Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
34.4	679.9	127.9	40343
46.6	1400	145.1	66994
53.5	2027	160.1	100445
59.1	2680		
67.5	4013	$\log P = A - B/(C + t/°C)$	
73,6	5306		P/mmHg
81.1	7333	A	6.83820
90.9	10919	B	1410.064
101.1	16212	C	195.639
115.6	27064		

*DTA—differential thermal analyzer

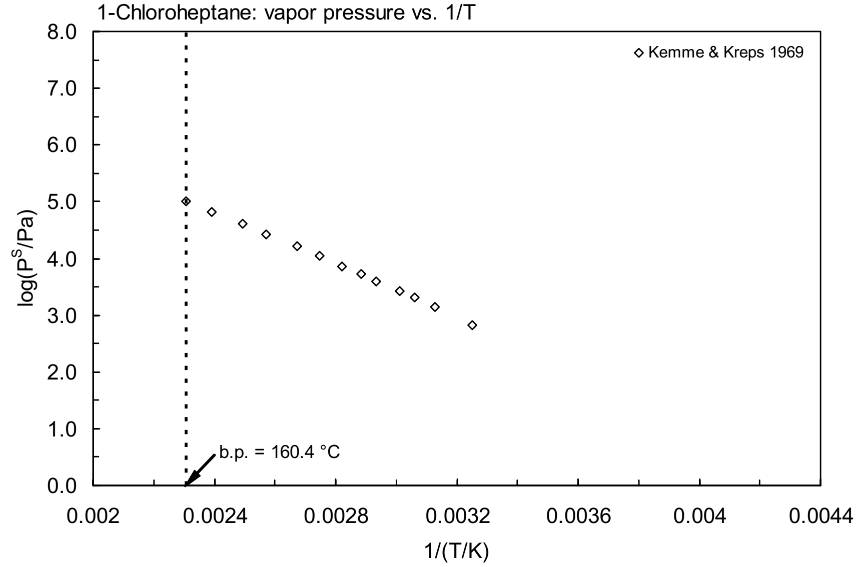
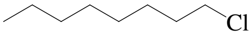


FIGURE 5.1.1.22.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chloroheptane.

5.1.1.23 1-Chlorooctane



Common Name: 1-Chlorooctane
Synonym: octyl chloride
Chemical Name: 1-chlorooctane
CAS Registry No: 111-85-3
Molecular Formula: $C_8H_{17}Cl$
Molecular Weight: 148.674
Melting Point (°C):
–57.8 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
183.5 (Lide 2003)
Density (g/cm^3):
0.8738, 0.8695 (20°C, 25°C, Dreisbach 1961; Weast 1982–83)
Molar Volume (cm^3/mol):
170.2 (15°C, calculated-density, Stephenson & Malanowski 1987)
205.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
53.25, 41.09 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
3.67* (generator column-GC, measured range 5–40°C, Sarraute et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
127 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 7.1231 – 1639.2/(204.2 + t/°C); temp range 86–231°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 7.1231 – 1369.20/(204.4 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
747* (54.1°C, differential thermal analysis, measured range 54.1–184.1°C, Kemme & Kreps 1969)
log (P/mmHg) = 6.84310 – 1469.829/(t/°C + 187.157); temp range 54.1–184.1°C (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)
118.2 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.17348 – 1598.257/(t/°C + 200.076) (Antoine eq. based on exptl. data of Kemme & Kreps 1969, temp range 54–184°C, Boublik et al. 1984)
log (P_L/kPa) = 5.968 – 1469.829/(T/K – 85.993); temp range 327–457 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 7.05152 – 1600.24/(t/°C + 200.28); temp range 64–184°C (Antoine eq., Dean 1992)
126.6* (calculated-Antoine eq. of Li & Rossini 1961, temp range 5–40°C, Saraute et al. 2004)

Henry's Law Constant (Pa·m^3/mol at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):
4437* (calculated-P/C, temp range 5–40°C, Sarraute et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
4.48 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

TABLE 5.1.1.23.1
Reported aqueous solubilities, vapor pressures and Henry's law constants of 1-chlorooctane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Aqueous solubility		Vapor pressure				Henry's law constant	
Sarraute et al. 2004		**Kemme & Kreps 1969**		**Sarraute et al. 2004**		**Sarraute et al. 2004**	
generator column-GC		**static method-DTA***		**extrapolated -Antoine eq.#**		**calculated-P/C**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
5.0	3.38	54.1	746.6	5.0	26.30	5.0	925
9.9	3.52	63.9	1307	9.9	39.55	9.9	1365
9.9	3.49	72.4	2040	9.9	39.71	9.9	1365
9.9	3.36	78.2	2706	9.9	39.71	9.9	1435
10.0	3.29	87.1	4040	10.0	40.04	10.0	1460
19.1	3.78	93.4	5346	19.1	81.99	19.1	2721
25.0	3.67	101.1	7359	25.0	126.6	25.0	4437
25.1	3.90	110.7	10732	25.1	127.1	25.1	4215
25.2	3.84	121.8	16159	25.2	128.0	25.2	4291
30.0	4.03	136.7	27798	30.0	179.8	30.0	5847
34.8	4.01	149.8	40210	34.8	248.4	34.8	8103
35.1	4.0	167.4	66795	35.1	252.5	35.1	8406
35.1	4.16	184.1	103085	35.1	252.5	35.1	8073
40.0	4.09			40.0	347.5	40.0	11429
		eq. 2	P/mmHg				
		A	6.84310	Antoine eq.			
		B	1469.829	#see Li & Rossini 1961			
		C	187.157	eq. 2	P/mmHg		
				A	7.1231		
				B	1369.20		
				C	204.4		
		pressure range 10–1500 torr mmHg					

*DTA—differential thermal analyzer

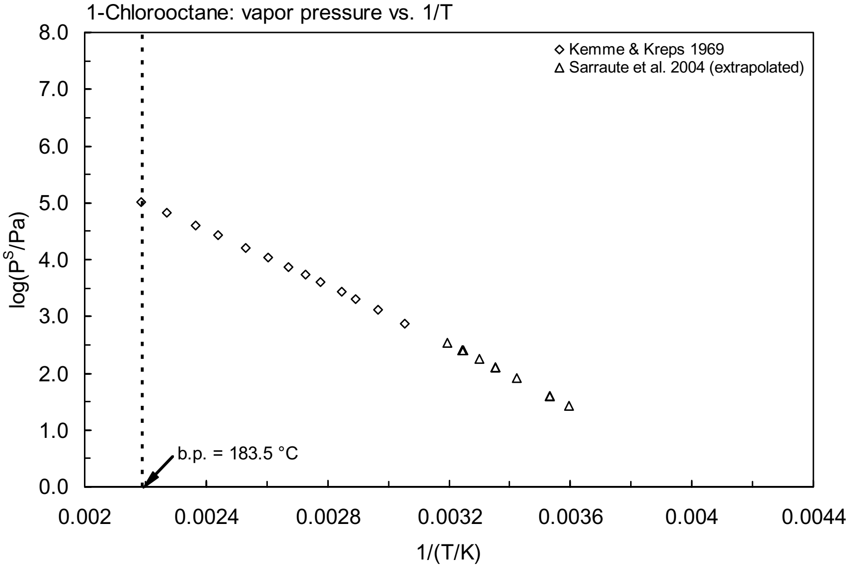
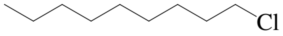


FIGURE 5.1.1.23.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorooctane.

5.1.1.24 1-Chlorononane



Common Name: 1-Chlorononane
Synonym: nonyl chloride
Chemical Name: 1-chlorononane
CAS Registry No: 2473-01-0
Molecular Formula: $C_9H_{19}Cl$
Molecular Weight: 162.700
Melting Point (°C):
 –39.4 (Dreisbach 1961; Weast 1982–83; Lide 2003)
Boiling Point (°C):
 205.2 (Lide 2003)
Density (g/cm^3):
 0.7886 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
 206.3 (20°C, calculated-density)
 228.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 58.27, 42.89 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 40.0 (extrapolated-Antoine eq., Dreisbach 1961)
 log (P/mmHg) = 7.1802 – 1736.11/(200.4 + t/°C); temp range 104–255°C (Antoine eq. for liquid state, Dreisbach 1961)
 log (P/mmHg) = 7.1802 – 1736.11/(200.4 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
 680* (69.1°C, differential thermal analysis, measured range 69.1–204.8°C, Kemme & Kreps 1969)
 log (P/mmHg) = 6.90463 – 1586.937/(t/°C + 185.505); temp range 69.1–204.8°C (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)
 35.9 (extrapolated-Antoine eq., Boublik et al. 1984)
 log (P/kPa) = 6.17172 – 1655.007/(t/°C + 205.166); temp range 69.1–204.8°C (Antoine eq., based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)
 log (P_L/kPa) = 6.09107 – 1332.89/(T/K – 54.65); temp range 289–409 K (Antoine eq., Stephenson & Malanowski 1987)
 log (P/mmHg) = 7.04654 – 1665.57/(t/°C + 192.26); temp range 69–205°C (Antoine eq., Dean 1992)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
 4.88 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives. $t_{½}$:
Half-Lives in the Environment:

TABLE 5.1.1.24.1
Reported vapor pressures of 1-chlorononane at various temperatures

Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
69.1	679.9	156.7	26731
70.8	733.3	170.3	40317
80.6	1280	188.6	66901
89.9	2013	204.8	100365
95.4	2613		
104.5	3933	log P = A – B/(C + t/°C)	
111.5	5280		P/mmHg
119.8	7333	A	6.94063
129.5	10626	B	1586.937
141.3	16159	C	185.505

*DTA—differential thermal analyzer

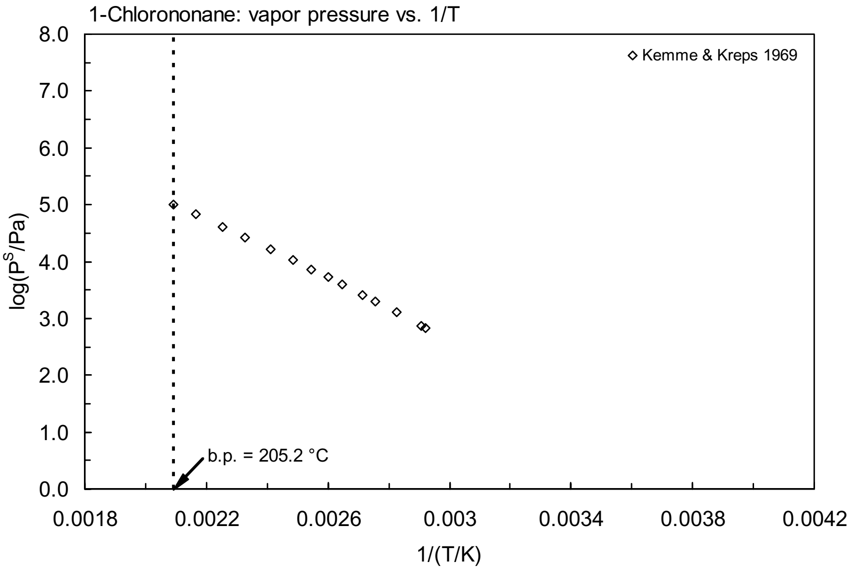
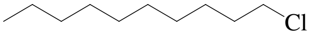


FIGURE 5.1.1.24.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorononane.

5.1.1.25 1-Chlorodecane



Common Name: 1-Chlorodecane
Synonym: decyl chloride
Chemical Name: 1-chlorodecane
CAS Registry No: 1002-69-3
Molecular Formula: $C_{10}H_{21}Cl$
Molecular Weight: 176.727
Melting Point (°C):
–31.3 (Dreisbach 1961; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
225.9 (Lide 2003)
Density (g/cm^3):
0.8705, 0.8666 (20°C, 25°C, Dreisbach 1961)
Molar Volume (cm^3/mol):
203.0 (20°C, calculated-density, Stephenson & Malanowski 1987)
250.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
63.35, 45.2 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
13.3 (calculated-Antoine eq., Dreisbach 1961)
$\log (P/mmHg) = 7.2372 - 1829.68/(196.6 + t/°C)$; temp range 121–278°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = 7.2372 - 1829.68/(196.6 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
733* (86.2°C, differential thermal analysis, measured range 86.2–225.6°C, Kemme & Kreps 1969)
$\log (P/mmHg) = 6.99172 - 1676.793/(t/°C + 182.017)$; temp range 86.2–225.6°C (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)
9.85 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 6.07379 - 1645.521/(t/°C + 178.639)$; temp range 86.2–225.6°C (Antoine eq. based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)
$\log (P_L/kPa) = 6.11662 - 1676.793/(T/K - 91.133)$; temp range 359–499 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = 6.93986 - 1639.06/(t/°C + 177.04)$; temp range 86–225.9°C (Antoine eq., Dean 1992)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.29 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:

TABLE 5.1.1.25.1
Reported vapor pressures of 1-chlorodecane at various temperatures

Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
86.2	733.3	189.5	40183
98.9	1400	208.6	66861
106.2	2000	225.6	100618
112.8	2693		
122.7	4106	log P = A – B/(C + t/°C)	
129.2	5346		P/mmHg
137.1	7293	A	6.99172
147.7	10666	B	1676.793
159.3	16065	C	182.017
175.7	26878		

*DTA—differential thermal analyzer

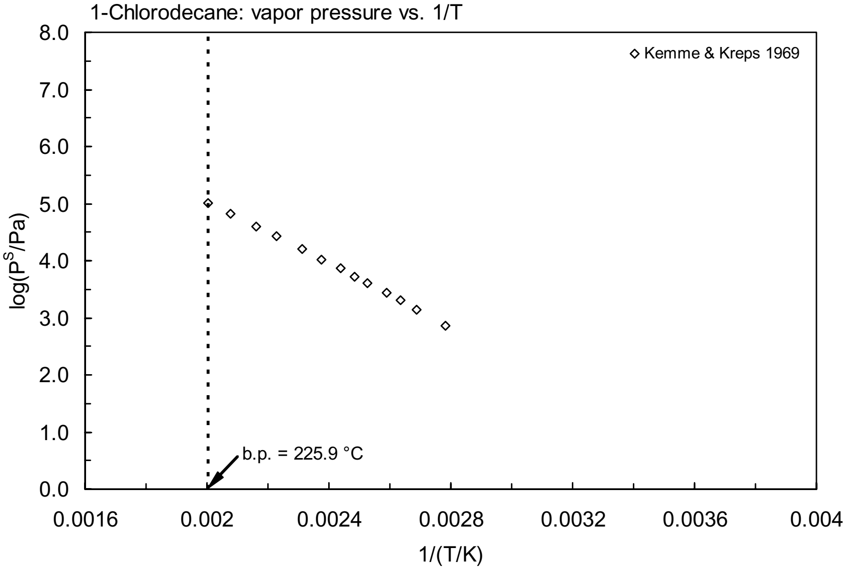
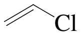


FIGURE 5.1.1.25.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorodecane.

5.1.1.26 Chloroethene (Vinyl chloride)



Common Name: Vinyl Chloride
Synonym: chloroethene, chloroethylene, monochloroethylene, monovinylchloride, MVC
Chemical Name: chloroethylene, vinyl chloride, chloroethene
CAS Registry No: 75-01-4
Molecular Formula: C_2H_3Cl, $H_2C = CHCl$
Molecular Weight: 62.498
Melting Point (°C):
–153.84 (Lide 2003)
Boiling Point (°C):
–13.8 (Lide 2003)
Density (g/cm^3 at 20°C):
0.9106 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
68.5 (20°C, Stephenson & Malanowski 1987)
65.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
18.636, 20.799 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
4.745 (Dreisbach 1959; quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
8720, 9000 (15, 30°C, shake flask-interferometry, Gross & Saylor 1931)
2700* (continuous solvent flow system at 1 atmospheric pressure, measured range 0.2–75°C, Hayduk & Laudie 1974)
60 (10°C, Pearson & Connell 1975)
60, 2700 (10, 25°C, selected, Dilling 1977)
1100 (Verschueren 1977, 1983)
6800 (20°C, selected, Nathan 1978)
8700* (restatement of Hayduk & Laudie 1974, temp range 0.2–75°C at saturated pressure of vinyl chloride, DeLassus & Schmidt 1981)
8800* (26°C, solubility bomb-headspace GC, measured range 15–85°C at saturated pressure of vinyl chloride, DeLassus & Schmidt 1981)
2763* (recommended, temp range 0–175°C, Horvath 1982)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
538000* (Antoine eq. regression, temp range –105.6 to –13.8°C, Stull 1947)
354600 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.49712 – 783.4/(230.0 + t/°C), temp range –100 to 50°C (Antoine eq. for liquid state, Dreisbach 1959)
104698* (–13.00°C, ebulliometry, measured range –64.9 to –13.00°C, McDonald et al. 1959)
381600 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.88054 – 912.5/(242.0 + t/°C); temp range –73 to 46°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.86108 – 892.757/(238.099 + t/°C); temp range –64.9 to 13.0°C (Antoine eq. from ebulliometric measurements, McDonald et al. 1959)

172719* (0°C, temp range –59.4 to 0°C, Huccura & Mathieu 1967)
546800 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 6263.0/(T/K)] + 8.202782; temp range –105.1 to –13.8°C (Antoine eq., Weast 1972–73)
392800 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 6.89117 – 905.008/(239.475 + t/°C); temp range –64.9 to –13.0°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
309300 (Pearson & McConnell 1975)
log (P/mmHg) = 6.89117 – 905.01/(239.48 + t/°C); temp range –657 to –13°C (Antoine eq., Dean 1985, 1992)
log (P/kPa) = 5.98598 – 892.757/(238.099 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
387000 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.98598 – 892.757/(–35.051 + T/K); temp range 208–260 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.20198 – 556.26/(–85.385 + T/K); temp range 259–328 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 52.9654 – 2.5016 × 10^3/(T/K) – 17.914·log (T/K) + 1.0821 × 10^{-2}·(T/K) – 4.531 × 10^{-14}·$(T/K)^2$; temp range 119–432 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
5680 (exptl.-1/K_{AW} = C_W/C_A, Hine & Mookerjee 1975)
4723 (calculated-bond contribution method, Hine & Mookerjee 1975)
117705 (10°C, Pearson & McConnell 1975)
39660 (calculated-P/C, Neely 1976)
106590 (calculated-P/C, Dilling 1977)
2350 (calculated-P/C, Mackay & Shiu 1981)
2817* (24.8°C, EPICS-GC/FID, measured range 10.3–34.6°C, Gossett 1987)
ln [H/(atm m^3/mol)] = 7.385 – 3286/(T/K); temp range 10.3–34.6°C (EPICS measurements, Gossett 1987)
2685* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 6.138 – 2931/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
2271 (computed value, Yaws et al. 1991)
2172 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 4.119 – 1223/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
1.39 (calculated-π substituent const., Hansch et al. 1968)
0.60 (Callahan et al. 1979; Mills et al. 1982)
1.23 (calculated-fragment const., Mabey et al. 1982)
2.79 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
0.845 (estimated-S, Lyman et al. 1982)
0.756 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
3.04, 1.60, < 1.0 (activated sludge, *Chlorella fusca*, golden ide, Freitag et al. 1984)
0.068 (from USEPA 86, Yeh & Kastenberg 1991)

Sorption Partition Coefficient, log K_{OC}:
0.9138 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.748 (estimated-S, Lyman et al. 1982)
0.477 (soil, selected, Jury et al. 1990)
1.756 (quoted from USEPA 1986, Yeh & Kastenberg 1991)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 25 min from water, by rapidly stirring aqueous solutions in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al 1982)

$t_{½}$(exptl) = 27.6 min, $t_{½}$(calc) = 0.0054 min, 16.1 min from water at 10°C (Dilling 1977)

$t_{½}$ ~ 0.805 h for volatilization from a river of 1-m deep with a current of 3 m/s and wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989);

estimated $t_{½}$ ~ 2.5 h from water (Thomas 1982);

volatilization $t_{½}$ = 0.2 to 0.5 d from soil at 1 and 10 cm incorporation (Jury et al. 1984);

$t_{½}$ = 30 d, estimated volatilization from soil (Jury et al. 1990).

Photolysis: degrade rapidly in air by reaction with photochemically produced hydroxyl radicals with an estimated $t_{½}$ = 1.5 d (Perry et al. 1977; quoted, Howard 1989).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = 6.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 26°C (Perry et al. 1977)

photooxidation $t_{½}$ was reported to be a few hours in the troposphere (Callahan et al. 1979)

$k_{OH} = 6.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1979,1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{O3} = 6.5 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} at 295 K (Sanhueza et al. 1976; quoted, Atkinson & Carter 1984)

$k_{O3} = 2.3 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} at room temp. (Gay et al. 1976; quoted, Atkinson & Carter 1984)

$k_{O3} = 2.5 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1979,1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{OH} = 6.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, residence time of 1.8 d, loss of 42.6% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

k_{OH}(calc) = 3.9×10^{12} cm^3 mol^{-1} s^{-1}, and $k_{O3} = 1.2 \times 10^6$ cm^3 mol^{-1} s^{-1} at 300 K (Lyman 1982)

k < 10^8 M^{-1} h^{-1} for singlet oxygen and 3.0 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

$k_{O3} = (2.45 \pm 0.45) \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} at 298 K (Zhang et al. 1983; quoted, Atkinson & Carter 1984)

$k_{O3} = 2.5 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1}, $k_{OH} = 6.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Tuazon et al. 1984)

$k_{NO3} = (1.4 \pm 0.9) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 ± 1 K (Andersson & Ljungström 1989)

photooxidation $t_{½}$ = 9.7–97 h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

k_{OH}(calc) = 6.6×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 6.6×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{NO3} = (2.3 \pm 1.1) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} relative to ethene at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)

$k_{NO3} = 2.30 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} with a calculate atmospheric lifetime τ = 42 d, and $k_{OH} = 6.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with τ(calc) = 3.5 d and $k_{O3} = 2.5 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} with τ(calc) = 66 d at room temp. (Atkinson et al. 1987)

k_{OH}(calc) = 5.3×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 6.6×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{NO3} = (3.30 \pm 1.66) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 ± 1 K (quoted from Anderson & Ljungström 1989, Atkinson 1991)

$k_{NO3} = 4.45 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 1990)

$k_{NO3} = 4.3 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1991)

k_{OH}(calc) = 5.25×10^{-12} cm^3 molecule^{-1} s^{-1} (as per Atkinson 1987 and 1988, Müller & Klein 1991)

Hydrolysis: $t_{½}$ <10 yr (Callahan et al. 1979);

estimated acid-catalyzed rate constant of 3.30×10^{-12} mol^{-1} s^{-1} at pH 5 with calculated $t_{½} = 2 \times 10^{11}$ d (Wolfe 1980; quoted, Ma et al. 1990)

abiotic hydrolysis or dehydrohalogenation $t_{½}$ < 120 months (Olsen & Davis 1990).

Biodegradation: abiotic degradation rate constant of k = 6.6×10^{-12} cm^3 molecule^{-1} s^{-1} at 26°C determined in laboratory experiments for the vapor phase reaction with hydroxyl radicals (Perry et al. 1977; quoted, Howard 1989)

$t_{½}$(aq. aerobic) = 672–4320 h, based on aqueous screening test data (Freitag et al. 1984; Helfgott et al. 1977; quoted, Howard et al. 1991) greater than 99% degraded after 108 d under aerobic conditions and approximately 65% being mineralized to $^{14}CO_2$ under aerobic conditions (Davis & Carpenter 1990);

$t_{1/2}$(aq. anaerobic) = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} > 60$ d (Olsen & Davis 1990)

$t_{1/2}$(aerobic) = 28 d, $t_{1/2}$(anaerobic) = 110 d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2}$ = 11 wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2}$ = 0.24–2.4 h from air for the reaction with OH radical (Darnall et al. 1976);

photodecomposition $t_{1/2}$ = 4.3 h with NO under simulated atmospheric conditions (Dilling et al. 1976); estimated $t_{1/2}$ = 1.5 d, based on its photochemical reaction with OH radical in air (Perry et al. 1977; quoted, Howard 1989);

residence time of 1.8 d, loss of 42.6% in 1d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

$t_{1/2}$ = 9.7–97 h, based on measured rate for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetimes τ = 42 d for the reaction with NO_3 radical for a 12-h nighttime, average concn. of 2.4×10^9 molecule/cm^3, τ = 3.5 d for the reaction with OH radical for a 12-h average concn. of 1.0×10^6 molecule/cm^3, and τ = 66 d for the reaction with O_3 for a 24-h, average concn. of 7×10^{11} molecule/cm^3 (Atkinson et al. 1987).

Surface water: estimated $t_{1/2}$ = 0.805 h for volatilization from a river of 1 m deep with a current of 3 m/s and a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2}$ = 672–4320 h, based on aqueous screening test data (Freitag et al. 1984; Helfgott et al. 1977; quoted, Howard et al. 1991).

Ground water: $t_{1/2}$ = 1344–69000 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and an estimated half-life for anaerobic biodegradation from a ground water field study of chlorinated ethenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} < 10$ d (Ryan et al. 1988);

$t_{1/2}$ = 0.2 to 0.5 d for volatilization from soil at 1 and 10 cm incorporation (Jury et al. 1984; quoted, Howard 1989);

$t_{1/2}$ = 30 d, estimated volatilization loss from soil (Jury et al. 1990);

$t_{1/2}$ = 30–180 d (Howard et al. 1991; quoted, Jury et al. 1992);

$t_{1/2}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} < 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988; quoted, Jury et al. 1992).

TABLE 5.1.1.26.1
Reported aqueous solubilities of chloroethene (vinyl chloride) at various temperatures

Hayduk & Laudie 1974		DeLassus & Schmidt 1981		DeLassus & Schmidt 1981		Horvath 1982	
compressibility apparatus		"restatement" data#		solubility bomb-GC/FID		summary of literature data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
at 1.0 atm							
0.2	7537	0.2	9000	15	9500	0	5460.
25	2700	25	8700	16	9950	25	2764
50	1278	50	10100	20.5	9150	50	1421
75	507	75	12800	26	8800	75	780
at 1.36 atm				29.5	8900	100	538
0.2	8438	# "restatement" data		35	9400	150	337
at 3.06 atm		from Hayduk & Laudie 1974		41	8900	175	320
25	7153			46.5	8800		
50	3993			55	9500		
75	2125			65	9200		
at 6.12 atm				72.5	9800		
50	7674			80	10000		
75	4965			85	11200		
ΔH_{sol}/(kJ mol^{-1})							
25°C							

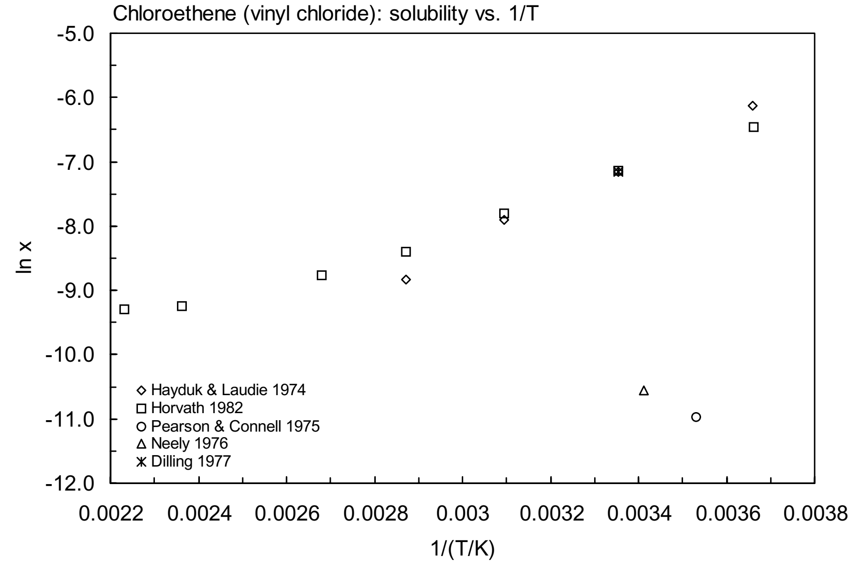


FIGURE 5.1.1.26.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for chloroethene.

TABLE 5.1.1.26.2
Reported vapor pressures of chloroethene (vinyl chloride) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log(T/K)$ (4)
$\log P = A - B/(T/K) - C\cdot(T/K) + D\cdot(T/K)^2$ (5)

Stull 1947		Huccura & Mathieu 1967		McDonald et al. 1959	
summary of literature data				ebullliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–103.6	133.3	–59.4	9870	–64.9	6769
–90.8	666.6	–54.3	13566	–56.4	12147
–83.7	1333	–49.4	18032	–43.37	25114
–75.7	2666	–44.5	23713	–29.09	51852
–66.8	5333	–39.5	31881	–14.83	97132
–61.1	7999	–34.5	39695	–13.64	102045
–53.2	13332	–29.65	50510	–13.00	104698
–41.3	26664	–24.9	63349		
–28.0	53329	–20.1	78440		
–13.8	101325	0.0	172719		
mp/°C	–153.7				

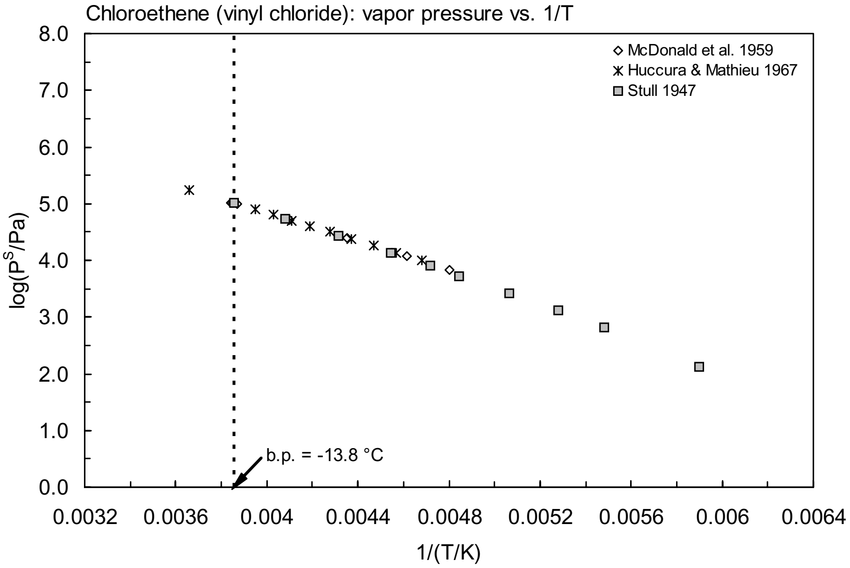


FIGURE 5.1.1.26.2 Logarithm of vapor pressure versus reciprocal temperature for chloroethene.

TABLE 5.1.1.26.3
Reported Henry's law constants of chloroethene (vinyl chloride) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)

$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)

$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)

$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$ (4) $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$ (4a)

$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

Hayduk & Laudie 1974		Gossett 1987		Ashworth et al. 1988	
compressibility measurement		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
at 1 atm					
0.2	834	10.3	1489	10	1520
25	2342	17.5	1956	15	1702
50	4348	24.8	2819	20	2199
75	7751	34.6	3627	25	2685
at 1.36 atm				30	3850
0.2	1018	eq. 4a	H/(atm m^3/mol)		
at 3.06 atm		A	7.385	eq. 4a	H/(atm m^3/mol)
25	2685	B	3286	A	6.138
50	4669			B	2931
75	7988				

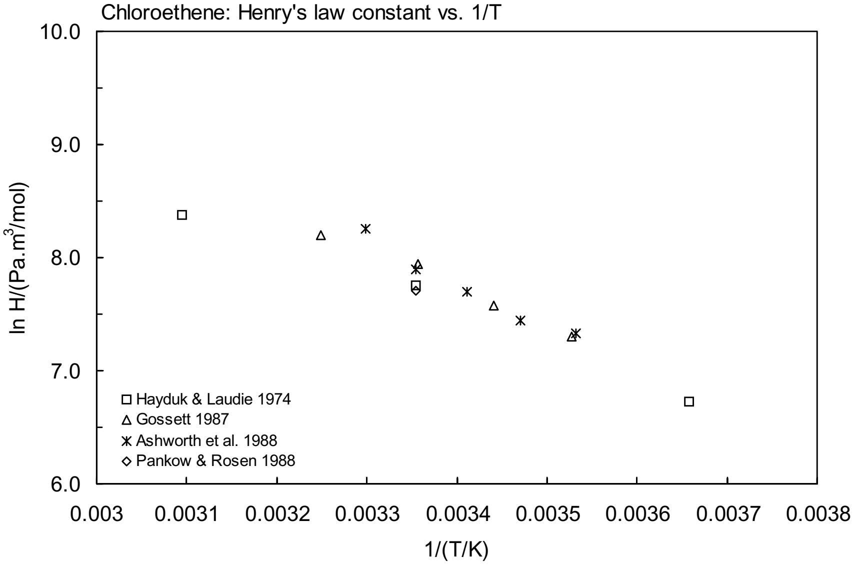
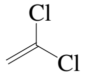


FIGURE 5.1.1.26.3 Logarithm of Henry's law constant versus reciprocal temperature for chloroethene.

5.1.1.27 1,1-Dichloroethene



Common Name: 1,1-Dichloroethene
Synonym: 1,1-dichloroethylene, vinylidene chloride, vinylidine chloride, 1,1-DCE
Chemical Name: 1,1-dichloroethene, 1,1-dichloroethylene
CAS Registry No: 75-35-4
Molecular Formula: $C_2H_2Cl_2$, $CH_2 = CCl_2$
Molecular Weight: 96.943
Melting Point (°C):
–122.56 (Lide 2003)
Boiling Point (°C):
31.6 (Lide 2003)
Density (g/cm^3 at 20°C):
1.2180 (Horvath 1982; Weast 1982–83; Verschueren 1983)
1.2132 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
79.9 (20°C, calculated-density)
86.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
26.49, 28.18 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
6.514 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
400 (20°C, shake flask-GC, McConnell et al. 1975; Pearson & McConnell 1975)
400 (20°C, literature average, Dilling 1977)
2250* (solubility bomb-headspace GC, measured range 15–90.5°C, DeLassus & Schmidt 1981)
210* (summary of literature data, Horvath 1982)
2640, 3675 (20°C, 30°C, saturation concn., Verschueren 1983)
2232 (30°C, headspace-GC, McNally & Grob 1984)
210 (Dean 1985; Riddick et al. 1986)
2843, 2790, 2782 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
2420* (recommended, temp range 0–90°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = $6.27413 - 3.8257 \times 10^{-2} \cdot (T/K) + 6.04607 \times 10^{-5} \cdot (T/K)^2$, temp range 288–363 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
86430* (Antoine eq. regression, temp range –77.2 to 31.7°C, Stull 1947)
97241* (30.39°C, ebulliometry, measured range –28.36 to 32.50°C, Hildebrand et al. 1959)
84500 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = $[-0.2185 \times 7211.8/(T/K)] + 8.087140$; temp range –77.2 to 31.7°C (Antoine eq., Weast 1972–73)
80040 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = $6.97215 - 1099.446/(237.184 + t/°C)$; temp range –28 to 32.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
79710 (literature average, Dilling 1977)
78780 (Verschueren 1977,1983)

80040 (interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.09904 – 1100.431/(237.274 + t/°C); temp range –28 to 32.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9722 – 1099.4/(237.2 + t/°C); temp range –28 to 32°C (Antoine eq., Dean 1985, 1992)
79860 (selected, Riddick et al. 1986)
log (P/kPa) = 6.10690 – 1104.29/(237.697 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
80060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.10046 – 1100.67/(–35.9 + T/K); temp range 244–306 K (Antoine eq., Stephenson & Malanowski 1987)
66190, 95740, 134520 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = –16.5419 – 1.6655 × 10^3/(T/K) + 13.923·log (T/K) – 4.0958 × 10^{-2}·(T/K) + 2.9995 × 10^{-5} · $(T/K)^2$; temp range 151–482 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3729 (20°C, batch stripping, Mackay et al. 1979)
3127* (24.3°C, equilibrium cell-concn ratio, measured range 2.5–26.1°C, Leighton & Calo 1981)
ln (k_H/atm) = 23.12 – 4618/(T/K); temp range 2.5–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
2649 (20°C, EPICS-GC, Linoff & Gossett 1983; Gossett 1985)
2645 (24.8°C, EPICS-GC, measured range 10–34.6°C, Gossett 1987)
ln [H/(atm m^3/mol)] = 8.845 – 3729/(T/K); temp range 10.0–34.6°C (EPICS measurements, Gossett 1987)
1520 (gas stripping-GC, Warner et al. 1987)
7529 (20°C, EPICS-GC, Yurteri et al. 1987)
2624* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 6.123 – 2907/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
19249 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
2316 (computed value, Yaws et al. 1991)
2320, 3415, 4813 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
2376 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 5.397 – 1586/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

2.13 (shake flask, Log P Database, Hansch & Leo 1987)
2.13 (recommended, Sangster 1993)
2.13 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.72 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

2.176 (calculated-K_{OW}, Kenaga & Goring 1980)
1.813 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$(exptl) ~ 22 min at 25°C for volatilization of 1 mg/L in water in an open container of 65-mm in depth stirring at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)
Evaporation $t_{1/2}$(exptl) = 27.2 min, $t_{1/2}$(calc) = 0.029 min, 20.1 min from water (Dilling 1977)
$t_{1/2}$(calc) = 5.9, 1.2, and 4.7 d from a pond, river, and lake, respectively, using data for the oxygen reaeration rate of typical bodies of water (Mill et al. 1982; quoted, Howard 1989).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{O3} = (3.7 ± 1.0) × 10^{-21} cm^3 $molecule^{-1}$ s^{-1} at 298 K (Hull et al. 1973; quoted, Atkinson & Carter 1984)
Photooxidation $t_{½}$ ~ 50 min reaction with NO_2 under UV irradiation (Gay, Jr. et al. 1976)
k < 10^8 M^{-1} h^{-1} for singlet oxygen and 3.0 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)
k_{OH} ~ 4.0 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, residence time of 2.9 d, loss of 29.2% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)
k ~10^3 M^{-1} s^{-1} for the reaction with ozone in water using 1.5 mM *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)
k_{O3} = 3.7 × 10^{-21} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Tuazon et al. 1984)
k_{OH} = (14.9 ± 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with reference to *n*-butane at 22.3 ± 1.2°C with a lifetime of 0.75 d and k_{OH} = 15.0 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with reference to *n*-pentane at 24.4 ± 0.4°C (relative rate method, Edney et al 1986)
photooxidation $t_{½}$ = 11 h in relatively clean air or under 2 h in polluted air (Howard 1989)
photooxidation $t_{½}$ = 9.9–98.7 h, based on measured rate data for the vapor phase reaction with OH radical in air (Goodman et al. 1986; quoted, Howard et al. 1991)
k_{NO3} = (6.60 ± 3.10) × 10^{-16} cm^3·$molecule^{-1}$ s^{-1} relative to ethene at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)
k_{NO3} = 6.6 × 10^{-16} cm^3·$molecule^{-1}$ s^{-1} with a calculated atmospheric lifetime of 15 d, k_{OH} = 8.1 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a lifetime of 3.4 d and k_{O3} = 3.7 × 10^{-21} cm^3 $molecule^{-1}$ s^{-1} with a lifetime of 12 yr at room temp. (Atkinson et al. 1987; quoted, Sabljic & Güsten 1990)
k_{OH}(calc) = 2.1 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 8.10 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1987)
k_{NO3} = 1.28 × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)
k_{NO3} = 1.23 × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K (Atkinson 1991)
k_{OH}(calc) = 2.04 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} (as per Atkinson 1987 and 1988, Müller & Klein 1991)
k_{OH}(calc) = 2.67 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = 10.9 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

Hydrolysis: estimated acid-catalyzed rate constant k = 1.4 × 10^{-13} mol^{-1} s^{-1} at pH 5 with $t_{½}$(calc) = 6 × 10^{12} d at pH 5 (Wolfe 1980);
estimated $t_{½}$ ~ 2.0 yr at pH 7.0 (Schmidt-Bleek et al. 1982; quoted, Howard 1989);
$t_{½}$ = 6–9 months has been observed with no significant difference in hydrolysis rate between pH 4.5 and 8.5 (Cline & Delfino 1987; quoted, Howard 1989);
abiotic hydrolysis or dehydrohalogenation half-life of 12 months (Olsen & Davis 1990).

Biodegradation: aerobic $t_{½}$(aq.) = 672–4320 h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); anaerobic $t_{½}$(aq.) = 1944–4152 h, based on anaerobic sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard 1989; Olsen & Davis 1990; Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{½}$ = 8.0 wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)
disappearance $t_{½}$ = 0.24–2.4 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
photodecomposition $t_{½}$ = 2.1 h with NO under simulated atmospheric conditions (Dilling et al. 1976);
residence time of 2.9 d, loss of 29.2% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
photooxidation $t_{½}$ = 11 h in relatively clean air (Edney et al. 1983; quoted, Howard 1989) or under 2 h in polluted air (Gay et al. 1976; quoted, Howard 1989);
lifetime of 0.75 d, based on measured rate data for the vapor phase reaction with OH radical in air at (22.3 ± 1.2)°C (Edney et al. 1986);
$t_{½}$ = 9.9–98.7 h, based on measured rate data for the vapor phase reaction with OH radical in air (Goodman et al. 1986; quoted, Howard et al. 1991);
atmospheric lifetimes: 15 d for the reaction with NO_3 radical for a 12-h nighttime average concn. of 2.4 × 10^9 molecule cm^{-3}, 3.4 d for the reaction with OH radical for a 12-h average concentration

of 1.0×10^6 molecule cm^{-3}, and 12 yr for the reaction with O_3 for a 24-h average concentration of 7×10^{11} molecule cm^{-3} at room temp. (Atkinson et al. 1987).

Surface water: $t_{½}$ = 672–4320 h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{½}$ = 1344–3168 h, based on estimated aqueous aerobic biodegradation half-life and anaerobic grab sample data for soil from ground water aquifer receiving landfill leachate (Wilson et al. 1986; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 672–4320 h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{½}$ < 10 d (Ryan et al. 1988).

Biota: $t_{½}$ < 10 d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.27.1
Reported aqueous solubilities of 1,1-dichloroethene at various temperatures

DeLassus & Schmidt 1981		Horvath 1982		Tse et al. 1992		Horvath & Getzen 1999a	
solubility bomb-GC/FID		summary of literature data		activity coefficient γ^∞ -GC		recommended, IUPAC-NIST	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
15	2400	20	300	20	2843	5	3100
17	2550	25	350	30	2790	10	2890
20.5	2500			40	2782	15	2700
25	2250					20	2550
28.5	2400					25	2420
29.5	2550					30	2330
38.5	2200					35	2260
45	2100					40	2230
51	2300					45	2220
55	2100					50	2250
60	2400					55	2300
65	2250					60	2390
71	2950					65	2510
74.5	2500					70	2650
81	2950					75	2830
85.5	3700					80	3040
90.5	3500					85	3280
						90	3550
						eq. 1	S/wt%
						temp range 288–363 K	

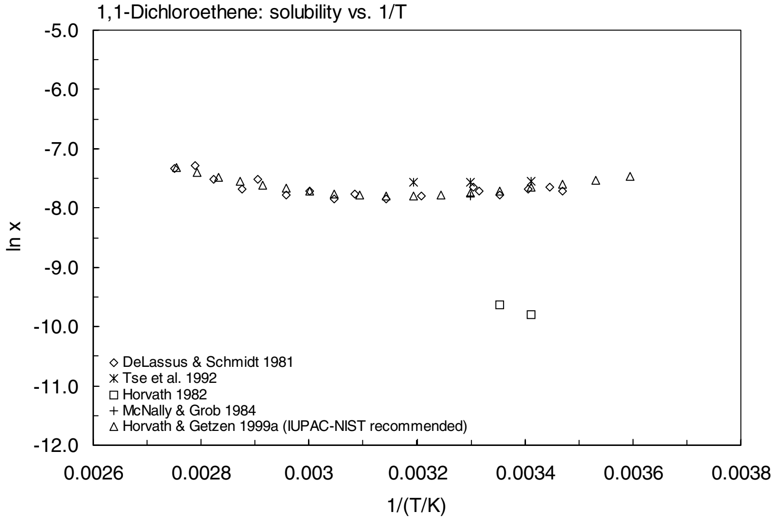


FIGURE 5.1.1.27.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,1-dichloroethene.

TABLE 5.1.1.27.2
Reported vapor pressures of 1,1-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log (T/K)$ (4)
$\log P = A - B/(T/K) - C\cdot(T/K) + D\cdot(T/K)^2$ (5)

Stull 1947		**Hildenbrand et al. 1959**	
summary of literature data		**ebulliometry**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**
–77.2	133.3	–28.36	6793
–60.0	666.6	–17.72	12204
–51.2	1333	–2.96	25279
–41.7	2666	13.75	51913
–31.1	5333	30.39	97241
–24.0	7999	31.56	101325
–15.0	13332	31.73	101986
–1.0	26664	32.50	104626
14.8	53329		
31.7	101325		
mp/°C	–122.5		

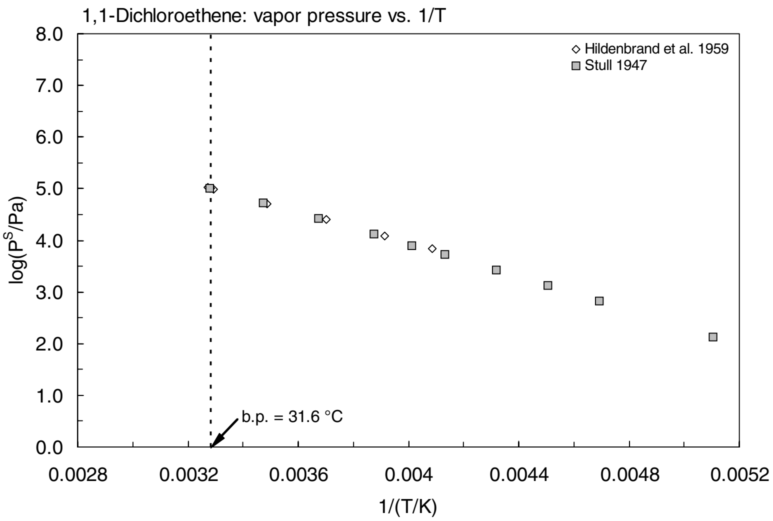


FIGURE 5.1.1.27.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1-dichloroethene.

TABLE 5.1.1.27.3
Reported Henry's law constants of 1,1-dichloroethene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm·m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B·(T/K) + C·(T/K)^2$	(5)		

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tse et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		activity coefficient γ^∞-GC	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
2.5	973	10.0	1287	10	1560	20	2320
7.0	1423	17.5	1935	15	2057	30	3415
12.9	2119	24.8	2645	20	2209	40	4813
18.0	2437	34.6	3708	25	2624		
19.5	3195			30	3222		
24.3	3127	eq. 4a	H/(atm m^3/mol)				
26.1	3914	A	8.845	eq. 4a	H/(atm m^3/mol)		
		B	3729	A	6.123		
eq. 3	H/atm			B	2907		
A	23.12						
B	4618						

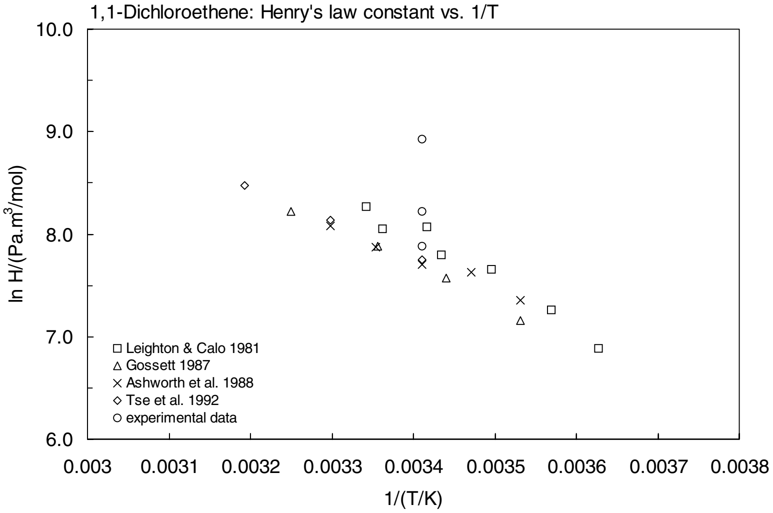
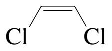


FIGURE 5.1.1.27.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1-dichloroethene.

5.1.1.28 *cis*-1,2-Dichloroethene



Common Name: *cis*-1,2-Dichloroethylene
Synonym: *cis*-acetylene dichloride, *cis*-1,2-dichloroethene, *cis*-1,2-dichloroethylene, (Z)-1,2-dichloroethene
Chemical Name: *cis*-1,2-dichloroethene, *cis*-1,2-dichloroethylene
CAS Registry No: 156-59-2
Molecular Formula: $C_2H_2Cl_2$, CHCl=CHCl
Molecular Weight: 96.943
Melting Point (°C):
–80.0 (Lide 2003)
Boiling Point (°C):
60.1 (Lide 2003)
Density (g/cm^3 at 20°C):
1.2837 (Horvath 1982; Weast 1982–83; Riddick et al. 1986)
1.2818 (Dean 1985)
Molar Volume (cm^3/mol):
75.52 (20°C, calculated-density)
86.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
31.57, 30.23 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
7.205 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3520 (Seidell 1940)
3500 (selected from literature or measured in DuPont laboratories, McGovern 1943)
5560 (37°C, shake flask-GC, Sato & Nakijima 1979)
3500 (summary of literature data, Horvath 1982)
7700 (Dean 1985)
6575, 6707, 6674 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
6292, 6092, 6220 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
6608 (20°C, limiting activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
6410* (tentative values, measured range 10–40°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
$S/(wt\%) = 27.7353 - 0.178316\cdot(T/K) + 2.93282 \times 10^{-4}\cdot(T/K)^2$, temp range 283–313 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
25571* (23.74°C, temp range 0.76–83.63°C, Ketelaar et al. 1947)
27260* (interpolated-Antoine eq. regression, temp range –58.4 to 59°C, Stull 1947)
28984* (dynamic-ebulliometry, measured range 19.2–62°C, Flom et al. 1951)
23540 (calculated-Antoine eq., Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 7420.6/(T/K)] + 7.685137$; temp range –58.4 to 260°C (Antoine eq., Weast 1972–73)
27010 (calculated-Antoine eq., Boublik et al. 1973)
$\log (P/mmHg) = 7.0233 - 1105.436/(230.62 + t/°C)$; temp range 0.76–83°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
27010, 26740 (interpolated-Antoine equations; Boublik et al. 1984)
$\log (P/kPa) = 6.14603 - 1204.804/(230.55 + t/°C)$; temp range 0.76–83.63°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 6.03144 - 1153.738/(222.905 + t/°C)$; temp range 19.2–62°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (P/mmHg) = 7.0223 - 1205.4/(230.6 + t/°C)$; temp range 0–84°C (Antoine eq., Dean 1985, 1992)
26700 (selected, Riddick et al. 1986)
$\log (P/kPa) = 6.9771 - 1651.52/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)
26980 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.30025 - 1293.95/(-32.41 + T/K)$; temp range 273–334 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.22178 - 1271.55/(-30.557 + T/K)$; temp range 332–495 K (Antoine eq.-II, Stephenson & Malanowski 1987)
21710, 33305, 49350 (20, 30, 40°C, estimated, Tse et al. 1992)
$\log (P/mmHg) = 55.9403 - 3.1677 \times 10^3/(T/K) - 18.572 \cdot \log (T/K) + 9.8828 \times 10^{-3} \cdot (T/K) + 5.7644 \times 10^{-14} \cdot (T/K)^2$; temp range 193–527 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
342.2 (exptl.-$1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975;)
1970, 2370 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
444 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
413.4* (EPICS-GC, measured range 10.3–34.6°C, Gossett 1987)
$\ln [H/(atm\ m^3/mol)] = 8.479 - 4192/(T/K)$; temp range 10.3–34.6°C (EPICS measurements, Gossett 1987)
441.1 (20°C, EPICS, Yurteri et al. 1987)
460* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
$\ln [H/(atm \cdot m^3/mol)] = 5.164 - 3143/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
745.5 (computed value, Yaws et al. 1991)
324, 496, 740 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
331, 518, 751 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
319 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
674.5 (modified EPICS method-GC, Ryu & Park 1999)
341 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 4.464 - 1559/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
1.86 (shake flask, Hansch & Leo 1985, 1987)
1.86 (recommended, Sangster 1993)
1.85 (infinite dilution activity coefficient-GC, Tse & Sandler 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:
2.56 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
1.176 (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:
1.69 (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:
Volatilization: evaporation $t_{1/2}$ = 18 min from dilute aqueous solution (Dilling 1975);
Evaporation $t_{1/2}$(exptl) = 19.4 min, $t_{1/2}$(calc) = 0.75 min, 20.7 min from water (Dilling 1977);
$t_{1/2}$ = 19.4 min from a slowly stirred beaker 6.5 cm deep equivalent to $t_{1/2}$ = 5.0 h in a body of water 1 m deep (Dilling 1977; quoted, Verschueren 1983; Howard 1990)
$t_{1/2}$ = 3.1 h was estimated from Henry's law constant for a model river 1 m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).
Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O3} = 6.2 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} at 296 K (Blume et al. 1976; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{OH} = 4.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, residence time of 2.9 d, loss of 29.2% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{O3} < 5.0 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{O3} = 3.7 \times 10^4$ cm^3 mol^{-1} s^{-1}, was estimated at 300 K (Lyman 1982)

k < 800 M^{-1} s^{-1} for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{O3} = 6.2 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} at room temp. (Tuazon et al. 1984)

photooxidation $t_{1/2}$ = 286 h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{NO3} = (7.5 \pm 3.5) \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}, relative to ethene at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)

$k_{NO3} = 7.5 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} with a calculated atmospheric lifetime of 130 d, $k_{OH} = 2.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with a lifetime of 12 d, and $k_{O3} < 5 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} with a lifetime of > 9 yr at room temp. (Atkinson et al. 1987)

k_{OH}(calc) = 2.2×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 2.38×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{NO3} = 1.46 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{OH} = (2.38 \pm 0.14) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Tuazon et al. 1988)

$k_{NO3} = (1.39 \pm 0.13) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (Atkinson 1991)

k_{OH}(calc) = 2.24×10^{-12} cm^3 molecule^{-1} s^{-1} (as per Atkinson 1987 and 1988, Müller & Klein 1991)

k_{O3}(aq.) = (310 ± 20) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2, with $t_{1/2}$ = 1.8 min at pH 7 and 25°C (Yao & Haag 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2}$ = 672–4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); anaerobic $t_{1/2}$ = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2}$ > 60 d (Wood et al. 1985; quoted, Olsen & Davis 1990);

k = = 0.74 yr^{-1} with $t_{1/2}$ = 88–339 d (Barrio-Lage et al. 1986; quoted, Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 0.24–2.4 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

Photooxidation $t_{1/2}$ ~100 min for reaction with NO_2 under UV irradiation, isomer not specified (Gay, Jr., et al. 1976)

photodecomposition $t_{1/2}$ = 3.0 h with NO and 3.0 h with NO_2 under simulated atmospheric conditions (Dilling et al. 1976);

residence time of 2.9 d, loss of 29.2% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2}$ = 129 d resulting from the ozone attacking of the double bond (Tuazon et al. 1984; quoted, Howard 1990);

$t_{1/2}$ = 8.0 d in the atmosphere for the reaction with photochemically produced OH radical (Goodman et al. 1986; quoted, Howard 1990);

$t_{1/2}$ = 286 h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric lifetimes: 130 d for the reaction with NO_3 radical for a 12-h nighttime average concn. of 2.4×10^9 molecule cm^{-3}, 12 d for the reaction with OH radical for a 12-h average concn. of 1.0×10^6 molecule cm^{-3}, and > 9.0 yr for the reaction with O_3 for a 24-h average concn. of 7×10^{11} molecule cm^{-3}, (Atkinson et al. 1987).

Surface water: $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

k(exptl) = (310 ± 20) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 25°C, with $t_{½}$ = 1.80 min at pH 7 (Yao & Haag 1991).

Ground water: 1344–69000 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991) and an estimated half-life for anaerobic biodegradation from a ground water field studies of chlorinated ethylenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.1.28.1
Reported aqueous solubilities of *cis*-1,2-dichloroethene at various temperatures

Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999	
activity coefficient γ^∞		activity coefficient γ^∞		IUPAC-NIST recommended	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	6575	20	6292	10	7550
30	6707	30	6092	15	7050
40	6674	40	6220	20	6670
				25	6410
				30	6310
				35	6360
				40	6560

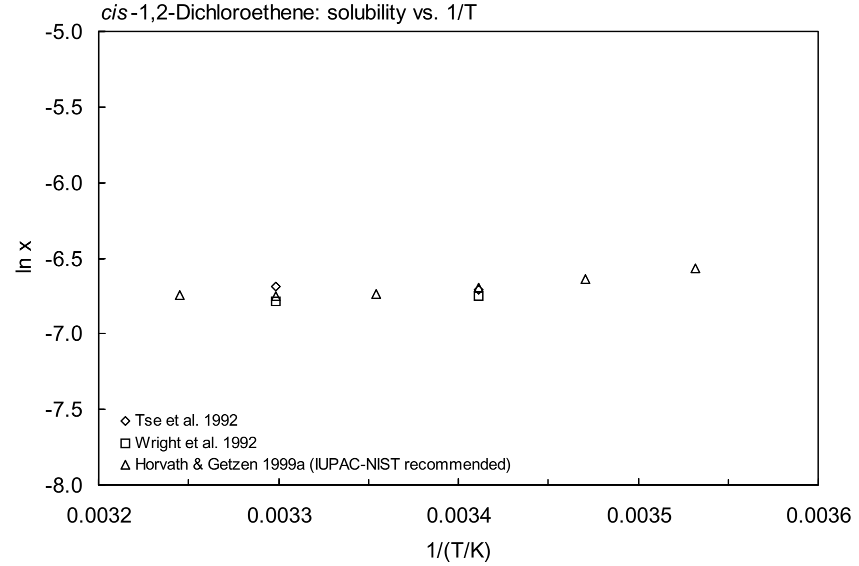


FIGURE 5.1.1.28.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *cis*-1,2-dichloroethene.

TABLE 5.1.1.28.2
Reported vapor pressures of *cis*-1,2-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		**Ketelaar et al. 1947*163**		**Flom et al. 1951**	
summary of literature data				**static method-manometer**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
–58.4	133.3	0.76	8626	19.2	20732
–39.2	666.6	1.68	9066	26.9	28984
–29.9	1333	3.85	10186	34.1	38957
–19.4	2666	6.45	11572	39.3	48143
–7.90	5333	10.73	14172	44.4	58035
–0.50	7999	15.03	17425	47.8	66048
9.50	13332	20.19	21865	52.1	76833
24.6	26664	23.74	25571	55.0	85206
41.0	53329	26.73	29051	58.4	954-5
59.0	101325	30.11	33344	60.4	101578
		36.35	42823	62.0	107924
mp/°C	–80.5	40.02	49316		
		45.52	60728		
		50.34	71980		
		55.28	85193		
		59.97	98992		
		62.85	109631		
		66.56	123149		
		71.84	145094		
		76.76	168039		
		83.63	283929		

*for a complete data set, see references.

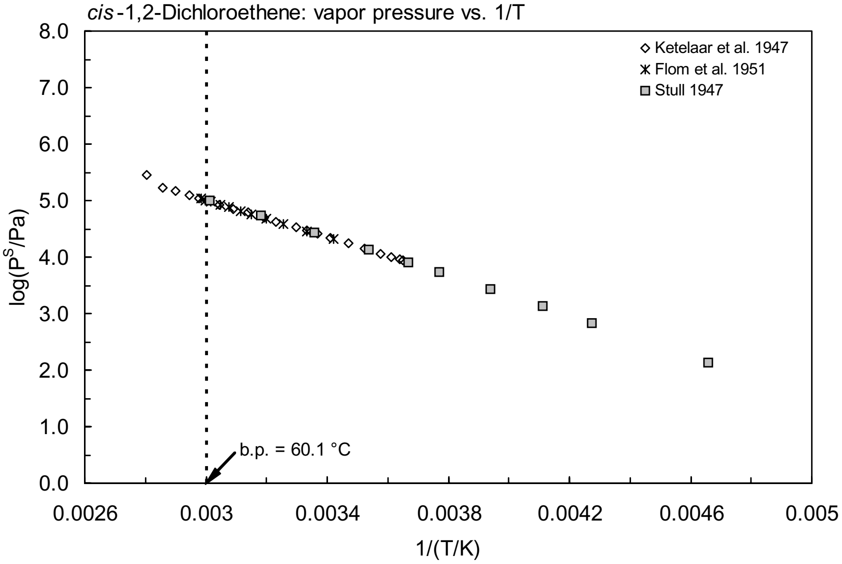


FIGURE 5.1.1.28.2 Logarithm of vapor pressure versus reciprocal temperature for *cis*-1,2-dichloroethene.

TABLE 5.1.1.28.3
Reported Henry's law constants of *cis*-1,2-dichloroethene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$ (4) $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$ (4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

Gossett 1987		**Ashworth et al. 1988**		**Tse et al. 1992**		**Wright et al. 1992**	
EPICS-GC		**EPICS-GC**		**activity coefficient γ^∞**		**activity coefficient γ^∞**	
t/°C	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**
10.3	174	10	273.6	20	324	20	331
17.5	268.5	15	330.3	30	496	30	518
24.8	413.4	20	364.8	40	740	40	751
34.6	552	25	460.0				
		30	582.6				
eq. 4a	H/(atm m³/mol)	eq. 4a	H/(atm m³/mol)				
A	8.479	A	5.164				
B	4192	B	3143				

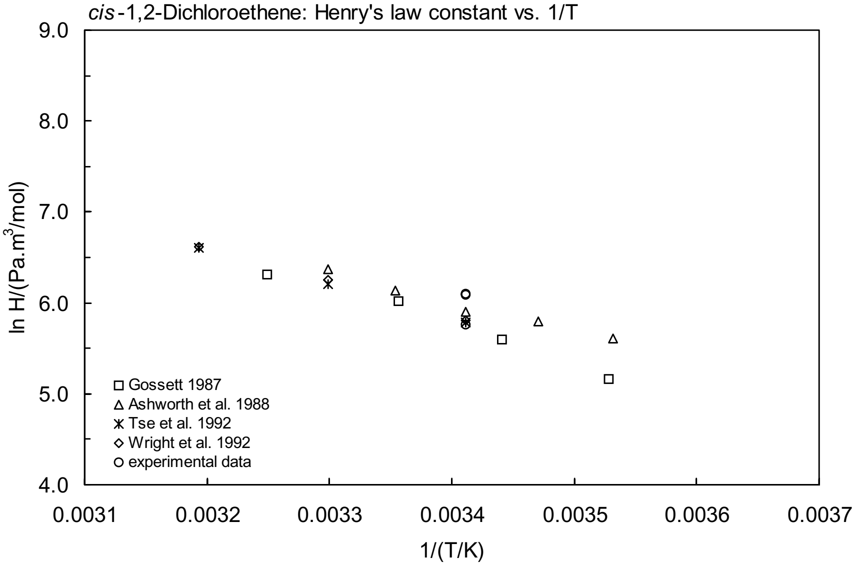
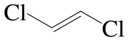


FIGURE 5.1.1.28.3 Logarithm of Henry's law constant versus reciprocal temperature for *cis*-1,2-dichloroethene.

5.1.1.29 *trans*-1,2-Dichloroethene



Common Name: *trans*-1,2-Dichloroethylene

Synonym: *trans*-1,2-dichloroethene, *trans*-1,2-dichloroethylene, *trans*-acetylene dichloride, Dioform, (E)-1,2-dichloroethene

Chemical Name: *trans*-1,2-dichloroethylene, *trans*-1,2-dichloroethene

CAS Registry No: 156-60-5

Molecular Formula: ClCH=CHCl

Molecular Weight: 96.943

Melting Point (°C):

–49.8 (Lide 2003)

Boiling Point (°C):

48.7 (Weast 1977,1982–83)

Density (g/cm^3 at 20°C):

1.2565 (Horvath 1982; Weast 1982–83)

Molar Volume (cm^3/mol):

77.2 (20°C, calculated-density)

86.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

36.04, 28.89 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.98 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6260 (Seidell 1940)

6300 (selected from literature of measured in DuPont laboratories, McGovern 1943; Dilling 1977)

6260 (recommended, Horvath 1982)

4480, 4480, 4333 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)

4488, 4111, 3931 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)

4488 (20°C, limiting activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

4520* (tentative values, temp range 10–40°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 7.803906 - 4.5457 \times 10^{-2} \cdot (T/K) + 6.96755 \times 10^{-4} \cdot (T/K)^2$, temp range 283–313 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

44649* (25.32°C, temp range –38.19 to 84.84°C, Ketelaar et al. 1947)

43180* (interpolated-Antoine eq. regression, temp range –65.4 to 47.8°C, Stull 1947)

42970* (25.2°C, dynamic-ebulliometry, measured range 13.5–51.6°C, Flom et al. 1951)

43470 (Hardie 1964)

36743 (calculated-Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 7243.1/(T/K)] + 7.748400$; temp range –65.4 to 236.5°C (Antoine eq., Weast 1972–73)

44190 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 6.96513 - 1141.984/(231.93 + t/°C)$; temp range –38 to 84°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

26660, 26660 (14, 20°C, Verschueren 1977, 1983)

40792* (23.138°C, temp range –0.68 to 46.721°C, Machat 1983; quoted, Boublik et al. 1984)

44190, 43960 (interpolated-Antoine equations, Boublik et al. 1984)

log (P/kPa) = 6.09105 – 1142.553/(231.998 + t/°C); temp range –38.2 to 84.84°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.04724 – 1112.321/(227.56 + t/°C); temp range –0.68 to 46.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9651 – 1141.9/(231.9 + t/°C); temp range –38.2 to 85°C (Antoine eq., Dean 1985, 1992)
45300 (selected, Riddick et al. 1986)
log (P/kPa) = 6.68147 – 1498.42/(T/K); temp range not specified (Antoine eq., Riddick et al. 1986)
44400 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.93307 – 1059.93/(–50.83 + T/K); temp range 263–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.27465 – 1226.69/(–33.653 + T/K); temp range 321–473 K (Antoine eq.-II, Stephenson & Malanowski 1987)
36250, 53970, 78100 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 48.4574 – 3.0496 × 10^3/(T/K) – 14.694·log (T/K) – 2.1262 × 10^{-9}·(T/K) + 7.3465 × 10^{-6}·$(T/K)^2$; temp range 223–508 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
682.7 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
1970, 2370 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
669 (calculated-P/C, Dilling 1977)
669 (calculated-P/C, Mackay & Shiu 1981)
950.5 (20°C, EPICS, Lincoff & Gossett 1983; Gossett 1985)
950* (EPICS-GC/FID, measured range 10–34.6°C, Gossett 1987)
ln [H/(atm m^3/mol)] = 9.341 – 4182/(T/K); temp range 10.0–34.6°C (EPICS measurements, Gossett 1987)
914 (20°C, EPICS-GC, Yurteri et al. 1987)
539 (gas stripping-GC, Warner et al. 1987)
958* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 5.333 – 2964/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
729 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
676 (computed value, Yaws et al. 1991)
800, 1196, 1793 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
768.7* (20°C, activity coeff. γ^∞-differential pressure transducer, measured range 20–40°C, Wright et al. 1992)
1023* (26.2°C, EPICS-GC, measured range 26.2–46.1°C, Hansen et al. 1993)
773 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
634.8 (modified EPICS method-GC, Ryu & Park 1999)
875 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 5.247 – 1669/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
2.06 (Hansch & Leo 1985)
2.09 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Hansch et al. 1995)
2.09 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
1.34 (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)
1.68 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
1.56 (calculated-$_{OW}$, Lyman et al. 1982; quoted, Howard 1990)
1.77 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{½}$:

Volatilization: experimental $t_{½}$(exptl) = 24 min for 1 mg/L from water when stirred at 200 rpm at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation $t_{½}$(exptl) = 24 min, $t_{½}$(calc) = 0.85 min, 20.8 min from water (Dilling 1977)

Volatilization $t_{½}$ = 3.0 h from a model river 1 m deep with 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O3} = 3.8 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} at 296 K (Blume et al. 1976; quoted, Atkinson & Carter 1984)

$k_{OH} = 4.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, residence time of 2.9 d, loss of 29.2% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{O3} = (1.8 \pm 0.29) \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} at 298 K (Zhang et al. 1983)

$k_{O3} = 1.2 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{O3} = 2.0 \times 10^{-23}$ cm^3 molecule^{-1} s^{-1} at 298 K, measured range 298–323 K (quoted, Atkinson & Carter 1984)

$k_{O3} = 2.3 \times 10^{5}$ cm^3 mol^{-1} s^{-1}, estimated at 300 K (Lyman 1982)

$k < 10^5$ M^{-1} h^{-1} for singlet oxygen and 6.0 M^{-1} h^{-1} for peroxy radicals at 25°C (Mabey et al. 1982)

$k = (5.7 \pm 1.0) \times 10^3$ M^{-1} s^{-1} for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{O3} = 1.8 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} at room temp. (Tuazon et al. 1984)

$k_{OH} = 1.79 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1986; quoted, Atkinson et al. 1987; Sabljic & Güsten 1990)

$k_{NO3} = (5.7 \pm 2.7)5 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{NO3} = 5.7 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} with a calculated atmospheric lifetime of 179 d, $k_{OH} = 1.8 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with a lifetime of 5.1 d and $k_{O3} = 1.5 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} with a lifetime of 110 d at room temp. (Atkinson et al. 1987)

k_{OH}(calc) = 2.5×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 1.8×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1987)

photooxidation $t_{½}$ = 25.2 h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{NO3} = 1.11 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{NO3} = (1.07 \pm 0.11) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} relative to ethene at 298 ± 2 K (Atkinson 1991)

k_{OH}(calc) = 2.57×10^{-12} cm^3 molecule^{-1} s^{-1} (as per Atkinson 1987 and 1988, Müller & Klein 1991)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{½}$ = 672–4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 2688–17280 h, based on estimated unacclimated aqueous aerobic degradation half-life (Howard et al. 1991);

k = 0.1 yr^{-1} with $t_{½}$ = 53 d (Wood et al. 1985; quoted, Olsen & Davis 1990);

rate constant k = 0.12–0.35 mini^{-1} in a fixed-film, packed-bed bioreactor containing a consortium of microorganisms (Strandberg et al. 1989);

k = 1.8 yr^{-1} with $t_{½}$ = 132–147 d (Barrio-Lage et al. 1986; quoted, Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 0.24–2.4 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

photodecomposition $t_{½}$ = 2.9 h with NO and $t_{½}$ = 2.8 h with NO_2 under simulated atmospheric conditions (Dilling et al. 1976);

Photooxidation $t_{½}$ ~ 100 min for reaction with NO_2 under UV irradiation, isomer not specified (Gay, Jr., et al. 1976) residence time of 2.9 d, loss of 29.2% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2}$ = 44 d resulting from ozone attacking of the double bond (Tuazon et al. 1984; quoted, Howard 1990);

$t_{1/2}$ = 3.6 d in the atmosphere for the reaction with photochemically produced OH radical (Goodman et al. 1986; quoted, Howard 1990);

$t_{1/2}$ = 25.2 h, based on estimated rate constant for reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric lifetimes, τ = 170 d for the reaction with NO_3 radical for a 12-h nighttime average concn. of 2.4×10^9 molecule cm^{-3}, τ = 5.1 d for the reaction with OH radical for a 12-h average concn. of 1.0×10^6 molecule·cm^{-3}, and τ = 110 d for the reaction with O_3 for a 24-h average concentration of 7×10^{11} molecule·cm^{-3} (Atkinson et al. 1987).

Surface water: $t_{1/2}$ = 672–4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2}$ = 1344–69000 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and estimated half-life for anaerobic biodegradation of chlorinated ethylenes from a ground water field study (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 672–4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2}$ < 10 d (Ryan et al. 1988).

Biota: $t_{1/2}$ < 10 d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.29.1
Reported aqueous solubilities of *trans*-1,2-dichloroethene at various temperatures

Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999	
activity coefficient γ^∞		activity coefficient γ^∞		IUPAC-NIST recommended	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	4480	20	4488	10	5250
30	4480	30	4111	15	4970
40	4333	40	3931	20	4720
				25	4520
				30	4330
				35	4190
				40	4080

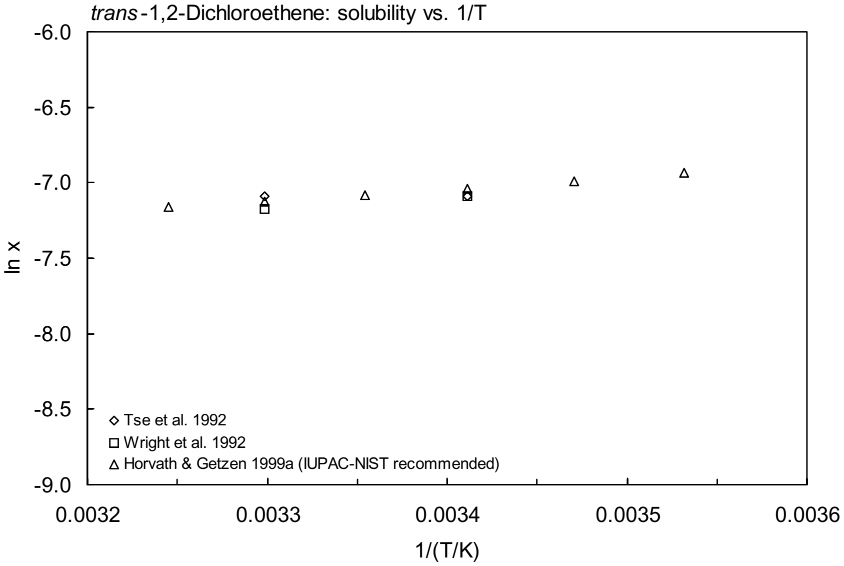


FIGURE 5.1.1.29.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *trans*-1,2-dichloroethene.

TABLE 5.1.1.29.2
Reported vapor pressures of *trans*-1,2-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C\cdot\log(T/K)$	(4)		

Stull 1947		Ketelaar et al. 1947*		Flom et al. 1951		Machat 1983, Thesis	
summary of literature data		in Boublik et al. 1984		static method-manometer		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–65.4	133.3	–38.19	1387	13.5	26131	–0.68	13944
–47.4	666.6	–28.3	3000	20.5	35210	3.154	16825
–38.0	1333	–15.12	6733	25.3	42956	7.12	20300
–28.0	2666	–7.29	10092	29.7	50836	11.306	24599
–17.0	5333	0.52	15086	34.7	61835	15.344	29372
–10.0	7999	5.98	19438	38.6	71581	19.302	34777
–0.20	13332	11.12	24718	41.6	79300	23.138	40792
14.3	26664	16.91	31651	44.1	86513	27.017	47616
30.8	53329	19.06	34757	46.8	95099	33.103	60215
47.8	101325	25.32	44649	49.1	102165	38.951	74768
		28.23	50329	51.6	111151	45.27	93376

TABLE 5.1.1.29.2 (*Continued*)

Stull 1947		**Ketelaar et al. 1947***		**Flom et al. 1951**		**Machat 1983, Thesis**	
summary of literature data				**static method-manometer**		**in Boublik et al. 1984**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
mp/°C	–122.5	32.15	38448			46.721	98149
		35.84	66888	$\Delta H_V/(kJ\ mol^{-1}) = 29.62$			
		43.72	88272			bp/°C	47.655
		47.17	99365			Antoine eq	
		48.83	105591			eq. 2	P/kPa
		50.82	112737			A	6.04724
		56.12	133389			B	1112.321
		63.58	167812			C	227.560
		68.19	192917				
		77.16	248619				
		84.84	304561				

*for a complete data set, see references.

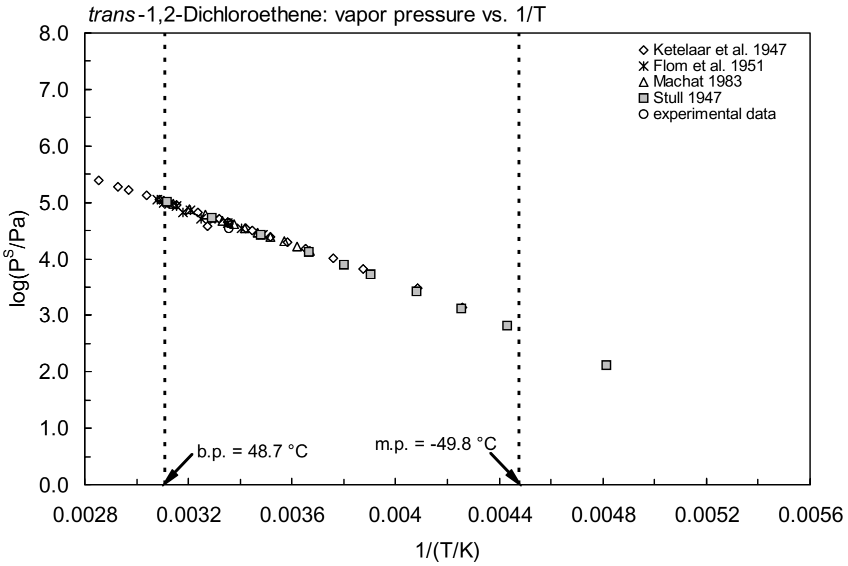


FIGURE 5.1.1.29.2 Logarithm of vapor pressure versus reciprocal temperature for *trans*-1,2-dichloroethene.

TABLE 5.1.1.29.3
Reported Henry's law constants of *trans*-1,2-dichloroethene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$ (4)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

$\log K_{AW} = A - B/(T/K)$ (1a)
$\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$ (4a)

Gossett 1987		**Ashworth et al. 1988**		**Tse et al. 1992**		**Hansen et al. 1993**	
EPICS-GC		**EPICS-GC**		**activity coeff. γ^∞ -GC**		**EPICS-GC**	
t/°C	**H/(Pa m^3/mol)**	**t/°C**	**H/(Pa m^3/mol)**	**t/°C**	**H/(Pa m^3/mol)**	**t/°C**	**H/(Pa m^3/mol)**
10.0	425.6	10	597.8	20	800	26.2	1023
17.5	668.7	15	714.3	30	1196	35.0	1591
24.8	950.4	20	868.4	40	1793	46.1	2087
34.6	1398.3	25	957.5				
		30	1226.0			eq. 4a	H/(kPa m^3/mol)
eq. 4a	H/(atm m^3/mol)			**Wright et al. 1992**		A	11 ± 1.96
A	9.341	eq. 4a	H/(atm m^3/mol)	**activity coeff. γ^∞**		B	3396 ± 602
B	4182	A	10.65	**t/°C**	**H/(Pa m^3/mol)**		
		B	4368				
				20	768.7		
				30	1238		
				40	1854		

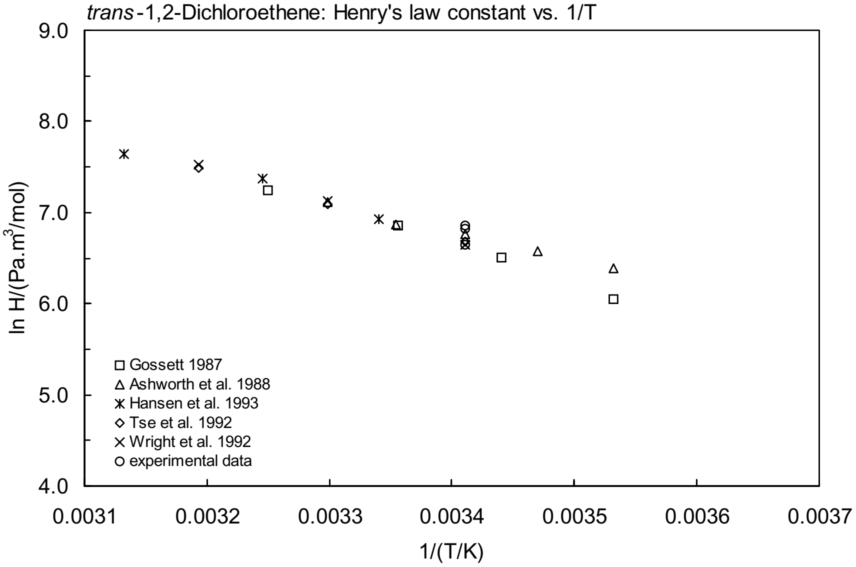
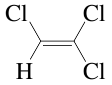


FIGURE 5.1.1.29.3 Logarithm of Henry's law constant versus reciprocal temperature for *trans*-1,2-dichloroethene.

5.1.1.30 Trichloroethylene



Common Name: Trichloroethylene
Synonym: TCE, acetylene trichloride, ethylene trichloride
Chemical Name: 1,1,2-trichloroethylene
CAS Registry No: 79-01-6
Molecular Formula: C_2HCl_3, $CHCl{=}CCl_2$
Molecular Weight: 131.388
Melting Point (°C):
 –84.7 (Lide 2003)
Boiling Point (°C):
 87.21 (Lide 2003)
Density (gm/cm^3 at 20°C):
 1.4642 (Dreisbach 1959; Horvath 1982; Weast 1982–83)
 1.4554 (25°C, Dreisbach 1959)
Molar Volume (cm^3/mol):
 89.02 (calculated-density, Miller et al. 1985)
 107.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 34.27, 31.47 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
 1818 (volumetric method, Wright & Schaffer 1932;)
 1100 (data presented in graph, temp range 0–80°C, McGovern 1943)
 1288* (temp range 10–50°C, Vallaud et al. 1957)
 1100 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
 1780, 1500, 1470 (3, 20, 34°C, shake flask-GC/ECD, Chiou & Freed 1977)
 1000, 1100, 1100 (1.5, 20, 25°C, literature average, Dilling 1977)
 1000 (shake flask-titration/turbidity, Coca et al. 1980)
 1472 (shake flask-LSC, Banerjee et al. 1980)
 1474 (shake flask-LSC, Veith et al. 1980)
 1100* (summary of literature data, temp range 0–80°C, Horvath 1982)
 1366 (generator column-HPLC, Tewari et al. 1982)
 743.1 (30°C, headspace-GC, McNally & Grob 1984)
 1370 (selected, Riddick et al. 1986)
 1421 (23–24°C, shake flask-GC, Broholm et al. 1992)
 1350 (20°C, calculated-activity coefficients, Wright et al. 1992)
 1483, 1450, 1468 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
 1349, 1409, 1308 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
 1300–1500 (9–71°C, generator column-GC, data presented in graph, Heron et al. 1998)
 1330 (20°C, limiting activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 1280* (recommended, temp range 0–60°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
 $S/(wt\%) = 1.4049 - 8.2223 \times 10^{-3}\cdot(T/K) + 1.3218 \times 10^{-5}\cdot(T/K)^2$, temp range 273–333 K (equation derived from literature solubility data, Horvath & Getzen 1999a)
 1417* (21°C, batch equilibrium-GC, sample prepared at 1.0 MPa, measure range 21–117°C, Knauss et al. 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19733* (temp range 25–87.15°C, Hertz & Rathmann 1912)
9331 (extrapolated, data presented in graph, McGovern 1943)
9645* (25.5°C, ebulliometry, measured range 18–86°C, McDonald 1944)
log (P/cmHg) = 30.482609 – 2936.227/(T/K) – 7.999975·log (T/K); temp range 18–86°C (ebulliometry, McDonald 1944)
9735* (interpolated-Antoine eq. regression, temp range 25–87.2°C, Stull 1947)
9906 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)
log (P/mmHg) = 7.02808 – 1315.0/(230.0 + t/°C); temp range 7–155°C (Antoine eq. for liquid state, Dreisbach 1959)
9723 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 8314.7/(T/K)] + 7.956342; temp range –43.8 to 86.7°C (Antoine eq., Weast 1972–73)
9224 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 6.51827 – 1018.603/(192.731 + t/°C); temp range 17–86°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
8000 (20°C, Perry & Chilton 1973)
7700 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
3066, 7866, 9866 (1.5, 20, 25°C, interpolated from literature data, Dilling 1977)
7998, 12660 (20°C, 30°C, Verschueren 1983; Hewitt et al. 1992)
9200, 9690 (interpolated-Antoine equations., Boublik et al. 1984)
log (P/kPa) = 5.59553 – 994.46/(189.705 + t/°C); temp range 17.8–86.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 4.70615 – 614.104/(140.089 + t/°C); temp range 25–87.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.5183 – 1018.6/(192.7 + t/°C); temp range 18–86°C (Antoine eq., Dean 1985, 1992)
6307 (selected, Riddick et al. 1986)
log (P/kPa) = 6.15298 – 1315.04/(230.0 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
9911 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.15298 – 1315.0/(–43.15 + T/K); temp range 280–428 K (Antoine eq., Stephenson & Malanowski 1987)
9691 (resistance measurement-Antoine eq., Foco et al. 1992)
7753, 12350, 19080 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = $23.6735 - 2.3763 \times 10^3/(T/K) - 5.8275\cdot\log(T/K) + 1.9586 \times 10^{-3}\cdot(T/K) + 2.8882 \times 10^{-14}\cdot(T/K)^2$; temp range 188–571 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1186 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
248, 1186 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)
967 (calculated-P/C, Neely 1976)
388.2, 1215 (1.5, 25°C, calculated-P/C, Dilling 1977)
890, 975 (20°C, exptl., calculated-P/C, Dilling 1977)
1103 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
log (H/atm) = 8.59 – 1716.16/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)
985 (20°C, batch stripping-GC, Mackay et al. 1979)
985* (25.2°C, equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)
ln (k_H/atm) = 21.89 – 4647/(T/K); temp range1.0–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
999 (20°C, batch stripping-GC, Munz & Roberts 1987)
970 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
774; 683 (20°C, EPICS-GC; batch air stripping-GC, measured range 10–30°C, Lincoff & Gossett 1984)
ln [H/(atm m^3/mol)] = 11.94 – 4929/(T/K); temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)
ln [H/(atm m^3/mol)] = 9.703 – 4308/(T/K); temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)

452, 795, 1348 (10, 20, 30°C, multiple equilibrium technique-GC, Munz 1985)
1185 (adsorption isotherm, Urano & Murata 1985)
970.7* (24.8°C, EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)
ln [H/(atm m^3/mol)] = 11.37 – 4780/(T/K); temp range 9.6–34.6°C (EPICS-GC, Gossett 1987)
816 (20°C, EPICS-GC, Munz & Roberts 1987)
log K_{AW} = 6.026 – 1909/(T/K); temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)
1185 (gas stripping-P/C, Warner et al. 1987)
1048 (20°C, EPICS, Yurteri et al. 1987)
1034* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 7.845 – 3702/(T/K); temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)
922 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
768.4 (purge and trap method, Tancrède & Yanagisawa 1990)
768* (tap water, EPICS-GC, measured range 25–47.2°C, Tancréde & Yanagisawa 1990)
log K_{AW} = 6.664 – 2141/(T/K); temp range 25–47.2°C (EPICS-GC, Tancréde & Yanagisawa 1990)
1182 (computed value, Yaws et al. 1991)
709, 1155, 1753 (20, 30, 40°C, determined from measured infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
756, 1152, 1908 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
996 (activity coefficient γ^∞ from gas stripping-GC, Li et al. 1993)
1043* (static headspace-GC, measured range 25–50°C, Robbins et al. 1993)
794 (23°C, batch air stripping-IR. Nielsen et al. 1994)
870* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)
381, 1073 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
ln K_{AW} = –3648/(T/K) + 0.00813·Z + 11.121; with Z salinity 0–35.5‰, temp range 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)
775 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
1180 (vapor-liquid equilibrium-GC, Turner et al. 1996)
K_{AW} = 0.151 – 0.00597·(T/K) + 0.000680·$(T/K)^2$; temp range 0–45°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)
751 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
885* (headspace equilibrium-GC, measured range 15–45°C, Peng & Wan 1997)
ln (k_H/atm) = 8.19 – 1642/(T/K); temp range 15–45°C (headspace-GC measurements, Peng & Wan 1997)
709* (20°C, headspace equilibrium-GC, Peng & Wan 1998)
1195 (sea water 36‰, headspace-GC, measured range 15–45°C, Peng & Wan 1998)
log (k_H/atm) = 8.62 – 1736/(T/K); sea water 36‰ NaCl, temp range: 15–45°C (headspace-GC measurements, Peng & Wan 1998)
1055 (modified EPICS method-GC, Ryu & Park 1999)
ln [H/(atm m^3/mol)] = 7.99 – 3736/(T/K); temp range 10–95°C (EPICS measurements, Heron et al. 1998)
1006; 981; 352 (EPICS-GC; quoted lit.; calculated-P/C, David et al. 2000)
703.4* (calculated from P and exptl measured solubility, temp range 21–117°C, Knauss et al. 2000)
823* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)
ln K_{AW} = 9.9697 – 3287.5/(T/K); measured range 15–4 0°C(SPME-GC, Bierwagen & Keller 2001)
765 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 5.874 – 1871/(T/K) (summary of literature data, Staudinger & Roberts 2001)
995* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
ln K_{AW} = 12.13 – 3908.2/(T/K); temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.37 (Hansch & Elkins 1971)
2.29 (Leo et al. 1971; Hansch & Leo 1979; 1987)
2.61 (shake flask-GC/ECD, Chiou & Freed 1977)
2.42 (shake flask-LSC, Banerjee et al. 1980)
2.42 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982; Veith et al. 1983)
2.86 (HPLC-k′ correlation, McDuffie 1981)

2.53 (generator column-HPLC, Tewari et al. 1982)
2.71, 2.79, 3.49, 3.57 (values used for OECD Lab. comparison tests, Harnisch et al. 1983)
2.84 (HPLC-RT correlation, Eadsforth 1986)
2.42 (recommended, Sangster 1993)
2.67 (calculated-activity coefficients γ^∞, Tse & Sandler 1994)
2.61 (recommended, Hansch et al. 1995)
2.27* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
2.99 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
1.59 (rainbow trout, Neely et al. 1974)
1.23–1.36 (calculated-K_{OW}, Veith et al. 1979; Veith et al. 1980)
1.23 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
1.23–1.59 (bluegill sunfish & rainbow trout, Barrows et al. 1980; Lyman 1981)
1.59 (rainbow trout, quoted, Bysshe 1982)
1.987 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
1.20 (calculated-MCI χ, Koch 1983)
2.996 (activated sludge, Freitag et al. 1984)
3.06, 2.39 (*Chlorella fusca*, calculated-K_{OW}, Geyer et al. 1984)
1.20, 1.05 (quoted, calculated, Sabljic 1987)
1.025 (quoted from USEPA 1986, Yeh & Kastenberg 1991)
1.420 (calculated-K_{OW}, McCarty et al. 1992)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
2.10 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
2.20 (Pavlou & Weston 1983,1984)
1.76, 2.20 (ICN humic acid-coated Al_2O_3, ICN humic acid, Garbarini & Lion 1985)
1.66; 2.14, 2.40 (predicted-S, predicted-K_{OW}, Garbarini & Lion 1985)
1.76; 0.616 (Sapsucker Woods humic acid, Sapsucker Woods fulvic acid, Garbarini & Lion 1986)
1.238, 2.079, 2.045, 0.30, 1.827 (tannic acid, lignin, zein, cellulose, Aldrich humic acid, Garbarini & Lion 1986)
2.025, 2.086 (Sapsucker Woods soil, Sapsucker Woods ether-extracted soil, Garbarini & Lion 1986)
2.161, 2.458 (humin, oxidized humin, Garbarini & Lion 1986)
2.663 (fats, waxes, resins, Garbarini & Lion 1986)
2.54, 1.72 (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
2.00; 1.84 (quoted from Seip et al. 1986, calculated-MCI χ, Bahnick & Doucette 1988)
2.03 (soil, Chiou et al. 1988; quoted, Grathwohl 1990)
2.02, 2.11 (soil: quoted, HPLC-RT correlation, Hodson & Williams 1988)
1.79 (20°C, humic acid, Peterson et al. 1988; quoted, Grathwohl 1990)
1.53 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.61, 2.12 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.89, 2.50, 2.25(organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.09; 2.56; 3.43(20°C, soil, sand and loess; weathered shale and mudrock; unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
1.97, 2.15 (20°C, calculated-K_{OW}, Grathwohl 1990)
0.30–3.64 (cellulose anthracite, quoted, Grathwohl 1990)
2.01 (calculated average, Olsen & Davis 1990)
2.20, 1.78 (humic acid, humic acid-coated Al_2O_3, Pavlostathis & Jaglal 1991)
2.03 (surface soil, Pavlostathis & Jaglal 1991)

3.39, 2.00 (organic carbon soil, Doust & Huang 1992)

1.60, 1.60, 2.15 (bentonite, green & tan clay, Doust & Huang 1992)

0.35, 1.40, 1.90, 2.20 (Barnwell, Congaree, McBean I & II sands, Doust & Huang 1992)

1.66, 2.64, 2.83 (calculated-equilibrium desorption data, Pavlostathis & Mathavan 1992)

2.23, 2.33, 2.35, 2.34, 2.34, 2.36, 2.41 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)

2.80; 2.00 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

1.92, 2.00, 1.75 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, $0.1 \leq$ OC $< 0.5\%$, average, Delle Site 2001)

Sorption Partition Coefficient, $\log K_{OM}$:

1.23 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

2.42, 1.89 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

2.78, 2.36 (organic cations treated Marlette soil B_t horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil B_t horizon OM 4.38%; Oshtemo soil B_t horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

1.74 (Florida peat, OC 57.1%, batch equilibrium-sorption isotherm, Rutherford & Chiou 1992)

Environment Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2}$(exptl.) = 21 min, calculated $t_{1/2}$(calc) = 0.48 min from dilute aqueous solution of 1 ppm initial concn. in a 250 mL beaker with constant stirring at room temp (Dilling et al. 1975);

volatilization k = 2.79, 5.07 g cm^{-2} s^{-1} at 23.7 ± 0.5°C into the atmosphere (Chiou & Freed 1977);

Evaporation $t_{1/2}$(exptl) = 17.7, 18.5, 23.5 min, $t_{1/2}$(calc) = : 0.47 min, 23.8 min at 20–25°C and $t_{1/2}$(exptl) = 31.9 min at 1.5°C from water (Dilling 1977)

ratio of evaporation rate constant to that of oxygen reaeration rate constant: measured as 0.49 as compared to the predicted 0.44 (Smith et al. 1980);

$t_{1/2}$(exptl) = 1.42×10^4 s and $t_{1/2}$(calc) = 5.1×10^3 s for water body of depth of 22.5 m (Klöpffer et al. 1982)

estimated $t_{1/2}$ = 3.4 h from water (Thomas 1982);

k = 0.025 d^{-1}, $t_{1/2}$ = 28 d in spring at 8–16°C, k = 0.052 d^{-1}, $t_{1/2}$ = 13 d in summer at 20–22°C, k = 0.045 d^{-1}, $t_{1/2}$ = 15 d in winter at 3–7°C for the periods when volatilization appears to dominate, and k = 0.064 d^{-1}, $t_{1/2}$ = 10.7 d with $HgCl_2$, and k = 0.081 d^{-1}, $t_{1/2}$ = 9.6 d without $HgCl_2$ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);

k = 7.22×10^{-3} h^{-1} (Mackay et al. 1985).

Photolysis: $t_{1/2}$ = 3.5 h estimated from lab. simulated UV photolysis (light intensity about 6 times of natural sunlight at noon on a summer day in Freeport) for 10 ppm to react with 5 ppm NO at 27 ± 1°C (Dilling et al. 1976);

probably would not occur (Callahan et al., 1979)

photocatalyzed mineralization by the presence of TiO_2 with the rate of 830 ppm $min^{-1} \cdot g^{-1}$ of catalyst (Ollis 1985);

k = (4.08–6.27) × 10^{-3} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = 2.0 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow system-LMR, Howard 1976)

Photooxidation $t_{1/2}$ ~ 120 min for reaction with NO_2 under UV irradiation (Gay, Jr. et al 1976)

$k_{OH}^* = (2.37 \pm 0.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 234–420 K (discharge flow-resonance fluorescence, Chang & Kaufman 1977)

$k_{OH} = (0.27 \pm 0.08) \times 10^{10}$ cm^3 M^{-1} s^{-1} at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1978)

$k_{OH} = 2.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson et al. 1979,1982; quoted, Tuazon et al. 1984; Atkinson et al. 1987)

$k_{OH} = 2.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, residence time of 5.3 d, loss of 17.2% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH} = 1.2 \times 10^{12}$ cm^3 mol^{-1} s^{-1} estimated, and $k_{O3} = 3.6 \times 10^3$ cm^3 mol^{-1} s^{-1} at 300 K (Lyman 1982)

$k_{O3} < 3 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} for the gas-phase reaction with ozone at 296 ± 2 K (Atkinson et al. 1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)
$k < 1000$ M^{-1} h^{-1} for singlet oxygen, $k = 6.0$ M^{-1} h^{-1} for RO_2 radical (Mabey et al. 1982)
$k = (17 \pm 4)$ M^{-1} s^{-1} for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)
$k_{O3} < 3 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1}, $k_{OH} = 2.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Tuazon et al. 1984)
k_{OH}(calc) = 1.4×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 2.4×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1985)
$k_{OH} = 2.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 0.10 d^{-1}, $k_{O3} < 3 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 0.002 d^{-1} at room temp. (Atkinson et al. 1985)
$k_{OH} = (2.86 \pm 0.40) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with reference to *n*-butane at 23.2 ± 1.1°C and a calculated atmospheric lifetime $\tau = 4.0$ d (Edney et al. 1986)
$k_{NO3} = (1.5 \pm 0.7) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Atkinson et al. 1987)
$k_{NO3} = 1.5 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} with a calculated atmospheric lifetime $\tau = 64$ d, $k_{OH} = 2.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with lifetime $\tau = 9.6$ d and $k_{O3} < 3 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} with lifetime $\tau > 1.5$ yr at room temp. (Atkinson et al. 1987)
k_{OH}(calc) = 0.70×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 2.36×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$k_{OH}* = 2.36 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)
k_{OH}(calc) = 6.92×10^{-13} cm^3 molecule^{-1} s^{-1} (as per Atkinson 1987 and 1988, Müller & Klein 1991)
$k_{NO3} = (2.81 \pm 0.17) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} relative to ethene at 298 ± 2 K (Atkinson 1991)
k(aq.) = (15 ± 2) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21 ± 1°C, with a half-life of 37 min at pH 7 (Yao & Haag 1991).

Hydrolysis: not an important process (Mabey et al. 1982);
$k = 0.065$ month^{-1} at 25°C with $t_{½} = 10.7$ months (Dilling et al. 1975; quoted, Howard et al. 1991);
$k = 9.0 \times 10^{-5}$ h^{-1} (Mackay et al. 1985);
abiotic hydrolysis or dehydrohalogenation $t_{½} = 10.7$ months (Olsen & Davis 1990)
$t_{½} = 320$ d at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: can be biodegraded by microorganisms in sea water;
$t_{½}$(aerobic) = 6 months to 1 yr based on acclimated soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991)
$k = 1.1$ yr^{-1} with $t_{½} = 230$ d (Roberts et al. 1982; quoted, Olsen & Davis 1990)
$t_{½}$(anaerobic) = 98 d to 4.5 yr, based on sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard et al. 1991);
$k = 0.06$ yr^{-1} with biodegradation $t_{½} = 33$ d, microcosm constructed with crushed rock and water containing low microbial biomass depleted all TCE in 21 months of incubation (Barrio-Lage et al. 1987, quoted, Olsen & Davis 1990)
$k \sim 0.02$ min^{-1} in a fixed-film, packed-bed bioreactor containing a consortium of microorganisms (Strandberg et al. 1989);
$k = 0.08$ yr^{-1} with $t_{½} = 43$ d (Olsen & Davis 1990)
$t_{½}$(aerobic) = 180 d, $t_{½}$(anaerobic) = 98 d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of 1×10^{-10} mL cell^{-1} h^{-1} for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:
$k_1 = 10.5$ h^{-1} (flagfish, calculated-BCF × k_2, McCarty et al. 1992)
$k_2 = 0.398$ h^{-1} (flagfish, estimated-one compartment first-order kinetics, McCarty et al. 1992)

Environmental Half-Lives:

Air: tropospheric $t_{½} = 6.0$ wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)
disappearance $t_{½} = 0.24$–2.4 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
photodecomposition $t_{½}$ = of 3.5 h with NO and $t_{½} = 2.9$ h with NO_2 under simulated atmospheric conditions (Dilling et al. 1976);
photooxidation $t_{½} \sim 120$ min for reaction with NO_2 under UV irradiation (Gay, Jr. et al. 1976)
residence time of 5.3 d, loss of 17.2% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2}$ = 27–272 h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetime $\tau = 4.0$ d, based on the photooxidation rate constant in the gas phase at 23.2 ± 1.1°C(Edney et al. 1986);

atmospheric lifetimes τ = 64 d for the reaction with NO_3 for a 12-h nighttime average concn. of 2.4×10^9 molecule/cm^3, τ = 9.6 d for the reaction with OH radical for a 12-h average concn. of 1.0×10^6 molecule cm^{-3}, and τ > 1.5 yr for the reaction with O_3 for a 24-h average concn. of 7×10^{11} molecule/cm^3 (Atkinson et al. 1987);

$t_{1/2}$ ~ 3.7 d (Yeh & Kastenberg 1991).

Surface water: estimated $t_{1/2}$ = 1.2–90 d in surface waters at various locations in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

half-lives from marine mesocosm: $t_{1/2}$ = 28 d in the spring at 8–16°C, $t_{1/2}$ = 13 d in the summer at 20–22°C and $t_{1/2}$ = 15 d in the winter at 3–7°C when volatilization dominates, and $t_{1/2}$ = 10.7 d and 8.6 d for experiments with and without $HgCl_2$ as poison, respectively, in September 9–15 (Wakeham et al. 1983)

Biodegradation $t_{1/2}$(aerobic) = 100 d, $t_{1/2}$(anaerobic) = 400 d; hydrolysis $t_{1/2}$ = 320 d at pH 7 in natural waters (Capel & Larson 1995)

$t_{1/2}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}$ ~ 90 d (Yeh & Kastenberg 1991);

measured rate constant k = (15 ± 2) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21 ± 1°C, with $t_{1/2}$ = 37 min at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2}$ = 7704–39672 h, based on hydrolysis half-life (Dilling et al. 1975; quoted, Howard et al. 1991) and anaerobic sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard et al. 1991)

$t_{1/2}$ ~ 2.0 yr in the ground water in the Netherlands (estimated, Zoeteman et al. 1981);

$t_{1/2}$ ~ 86 d (Yeh & Kastenberg 1991).

Soil: $t_{1/2}$ < 10 d (Ryan et al. 1988);

$t_{1/2}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}$ ~ 43 d in upper soil and $t_{1/2}$ ~ 86 d in lower soil (Yeh & Kastenberg 1991).

Sediment: $t_{1/2}$ ~ 43 d (estimated, Yeh & Kastenberg 1991).

Biota: $t_{1/2}$ < 1 d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{1/2}$ < 10 d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.30.1
Reported aqueous solubilities of trichloroethylene at various temperatures

$$S/(wt\%) = 0.10494 + 4.9038 \times 10^{-5}\cdot(t/°C) + 6.4541 \times 10^{-6}\cdot(t/°C)^2 - 1.8808 \times 10^{-8}\cdot(t/°C)^3 \quad (1)$$

$$S/(wt\%) = 1.4049 - 8.2223 \times 10^{-3}\cdot(T/K) + 1.3218 \times 10^{-5}\cdot(T/K)^2 \quad (2)$$

1.

Vallaud et al. 1957		Horvath 1982		Tse et al. 1992		Wright et al. 1992	
in Horvath 1982		summary of literature data		activity coefficient		activity coefficient	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
10	1280	0	1049	20	1483	20	1340
20	1285	10	1061	30	1450	30	1409
25	1288	20	1083	40	1468	40	1308
30	1290	25	1099				
40	1305	30	1117				
50	1330	40	1160				
		50	1212				
		60	1271				
		70	1335				
		80	1405				
		eq. 1	S/wt%				

(Continued)

TABLE 5.1.1.30.1 (*Continued*)

2.

Horvath & Getzen 1999a				Knauss et al. 2000	
summary of literature data				batch equilibrium-GC	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
				at 1.0 MPa	
0	1450	40	1260	21	1417
5	1410	45	1270	50	1450
10	1370	50	1280	75	1878
15	1330	55	1300	99	2872
20	1310	60	1330	117	5268
25	1280				
30	1279	eq. 2	S/wt%		
35	1260	temp range 273–333 K			

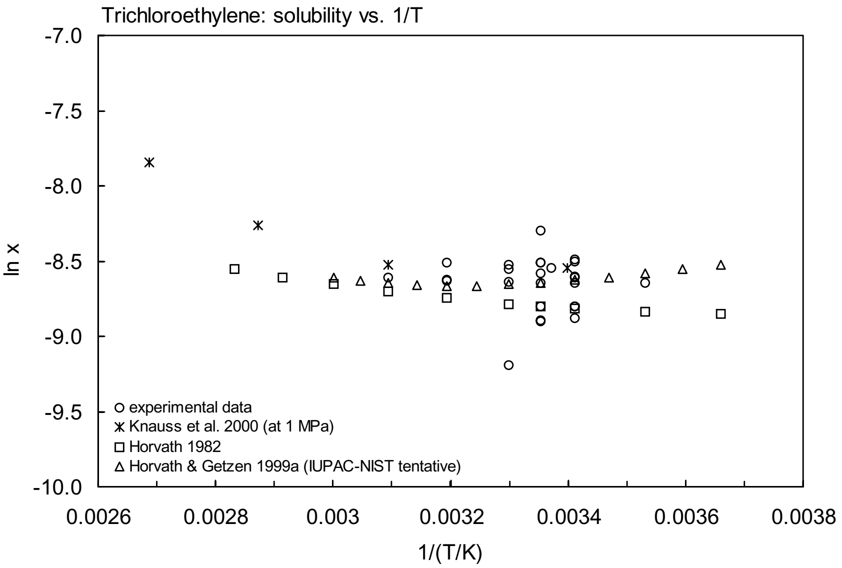


FIGURE 5.1.1.30.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.2
Reported vapor pressures of trichloroethylene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\qquad \ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\qquad \ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Hertz & Rathmann 1912		**McDonald 1944**		**Stull 1947**	
		ebulliometry		**summary of literature data**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
25.0	9733	17.8	4239	–43.8	133.3
30.0	12266	19.85	7226	–22.8	666.6
38.0	18532	20.99	7506	–12.4	1333
44.15	23598	24.4	8813	–1.0	2666
45.0	24398	25.5	9546	11.9	5333
51.0	31197	27.4	10319	20.0	7999
65.0	31329	30.2	11999	31.4	13332
77.0	74927	31.2	12426	48.0	26664
87.15	101325	34.39	14292	67.0	53329
		38.49	17305	86.7	101325
		39.29	18025		
		42.41	20545	mp/°C	–73
		44.51	22425		
		46.44	24318		
		51.05	29264		
		55.8	35210		
		60.5	41876		
		65.07	48889		
		71.44	61115		
		76.93	72988		
		80.38	81966		
		85.82	97018		
		86.47	98992		

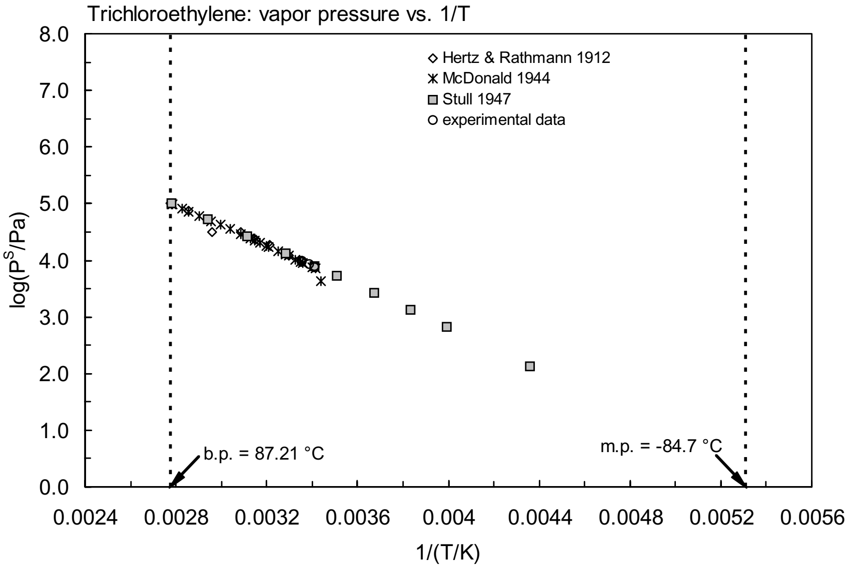


FIGURE 5.1.1.30.2 Logarithm of vapor pressure versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.3
Reported Henry's law constants of trichloroethylene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3) $\log (k_H/\text{atm}) = A - B/(T/K)$ (3a)
$\ln H = A - B/(T/K)$ (4) $\log H = A - B/(T/K)$ (4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

1.

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancréde & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.0	240	9.6	383	10	545.1	25	768
1.0	254.4	17.5	324.2	15	675.8	26.5	797.2
1.2	231.2	24.8	970.7	20	853.2	27.4	999.5
2.5	307.1	34.6	1510	25	1034	28.9	979.4
7.0	366.4			30	1297	28.9	828.7
10.0	424.4	eq. 4	H/(atm m³/mol)			29.7	881.2
12.0	464.7	A	11.37	eq. 4	H/(atm m³/mol)	29.9	1159
12.0	484.8	B	4780	A	7.845	33.3	1019
12.9	523.4			B	3702	35.6	1386
14.0	565.2					38.3	1554
18.0	683.9					40	1484
18.0	692.3					44.7	1638
18.0	683.9					45	2724
19.0	717.7					47.2	2504
19.2	761.1						

TABLE 5.1.1.30.3 (*Continued*)

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancréde & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
19.5	723.2					eq. 1a	K_{AW}
24.3	979.6					A	6.664
25.2	984.7					B	2141
25.3	995.3						
26.0	1005						
26.0	1028						
26.1	1018						
eq. 3	k_H/atm						
A	22.68						
B	4735						

2.

Tse et al. 1992		Wright et al. 1992		Robbins et al. 1993		Dewulf et al. 1995	
activity coefficient		activity coefficient		headspace-GC		EPICS-GC	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
20	709	20	756	25	1043	2.0	231.05
30	1155	30	1152	30	1330	6.0	290.1
40	1753	40	1753	40	1672	10.0	327.2
				45	2270	18.2	615.3
				50	2665	25.0	870.1
						eq. 1	K_{AW}
						A	11.121
						B	3648

3.

Peng & Wan 1997		Knauss et al. 2000		Bierwagen & Keller 2001		Görgényi et al. 2002	
static headspace-GC		calculated-P/C(measured)		SPME-GC		EPICS-SPME method	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/Pa m^3/mol
15	575	21	703.4	15	585	2.0	246
20	709	50	2552	25	823	6.0	348.6
25	885	75	4934	30	1114	10	447
30	1167	99	6854	40	1523	18	718
35	1309	117	6127			25	995
40	1650			eq 1	K_{AW}	30	1308
45	2005			A	9.9697	40	1871
				B	3287.5	50	2765
eq. 3	k_H/atm					60	3601
A	8.62						
B	1736					eq. 1	K_{AW}
						A	12.13
						B	3908.2

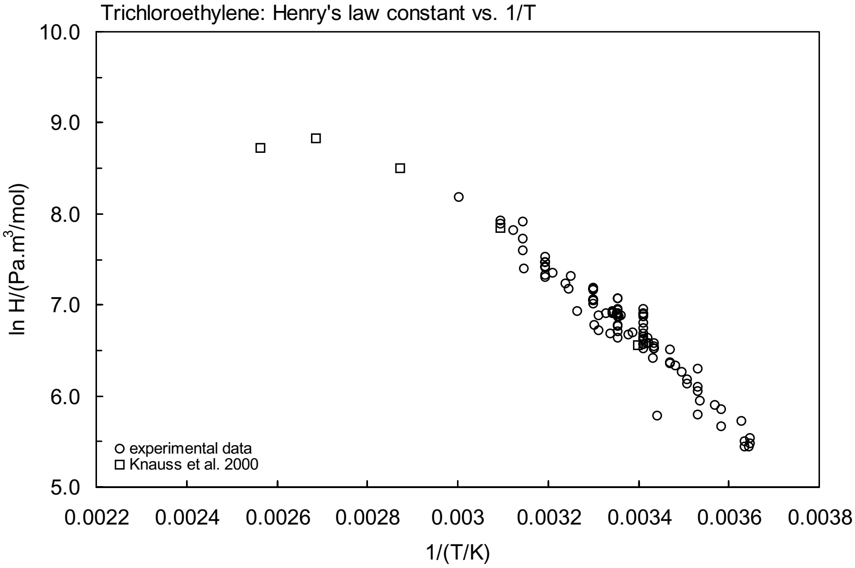


FIGURE 5.1.1.30.3 Logarithm of Henry's law constant versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.4
Reported octanol-water partition coefficients of trichloroethylene at various temperatures

Dewulf et al. 1999	
EPICS-GC	
t/°C	log K_{OW}
2.2	2.18
6.0	2.18
10.0	2.28
14.1	2.24
18.7	2.29
24.8	2.20

change in enthalpy:
ΔH_{OW}/(kJ mol^{-1}) = 3.4
(–8.4 to 15.2)
enthalpy of transfer
ΔH_{oct}/(kJ mol^{-1}) = 2.7
(–9.0 to 14.5)

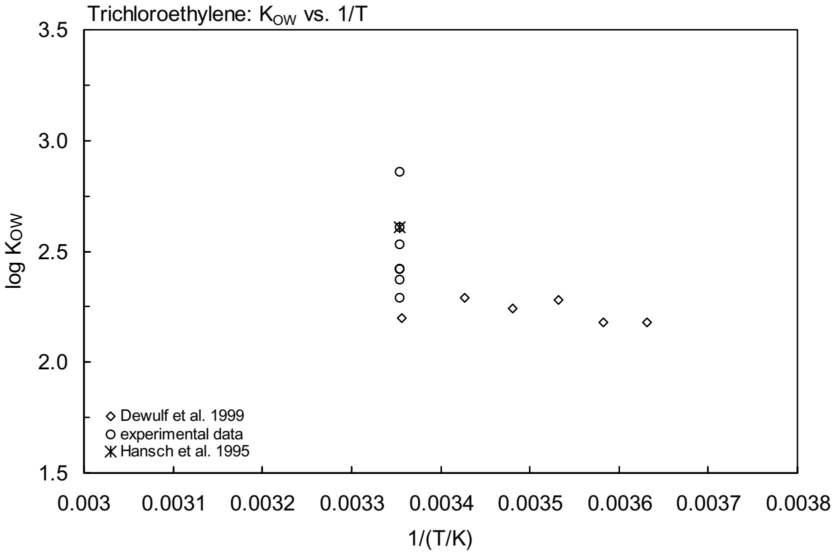
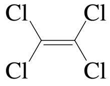


FIGURE 5.1.1.30.4 Logarithm of K_{OW} versus reciprocal temperature for trichloroethylene.

5.1.1.31 Tetrachloroethylene



Common Name: Tetrachloroethylene
Synonym: ethylene tetrachloride, perchloroethene, perchloroethylene, tetrachloroethene, 1,1,2,2-tetrachloro-ethylene
Chemical Name: tetrachloroethylene
CAS Registry No: 127-18-4
Molecular Formula: C_2Cl_4, $CCl_2{=}CCl_2$
Molecular Weight: 165.833
Melting Point (°C):
  –22.3 (Lide 2003)
Boiling Point (°C):
  121.3 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.62272, 1.61446 (20°C, 25°C, Dreisbach 1959)
  1.6227 (Horvath 1982; Weast 1982–83)
  1.62283, 1.61431 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
  102.0 (20°C, calculated-density)
  128.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  39.61, 34.72 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  10.56 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  150 (selected from literature or measured in DuPont laboratories, data also presented in graph, temp range 0–80°C, McGovern 1943)
  150 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
  130, 120, 140 (1.5, 20, 25°C, selected from literature, Dilling 1977)
  200 (20°C, shake flask-GC, Chiou et al. 1977)
  400 (shake flask-GC, Freed et al. 1979)
  136 (37°C, shake flask-GC, Sato & Nakijima 1979)
  486 (shake flask-LSC, Banerjee et al. 1980)
  200 (shake flask-titration/turbidity, Coca & Diaz 1980, Coca et al. 1980)
  478 (shake flask-LSC, Veith et al. 1980)
  150* (summary of literature data, temp range 0–80°C, Horvath 1982)
  242 (23–24°C, shake flask-GC, Broholm et al. 1992)
  286* (19.5°C, shake flask-GC/TC, measured range 0–91.8°C, Stephenson 1992)
  256 (activity coeff. by inert gas stripping-GC, Li et al. 1993)
  258.8 (20°C, limiting activity coeff. by inert air stripping-GC, Hovorka & Dohnal 1997)
  206* (tentative value, temp range 0–70°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
  $S/(wt\%) = 0.26479 - 1.5487 \times 10^{-3}\cdot(T/K) + 2.4477 \times 10^{-6}\cdot(T/K)^2$, temp range 273–343 K (equation derived from reported solubility data, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)
  192.3* (22°C, batch equilibrium-GC, sample prepared at 1.0 MPa, measure range 22–161°C, Knauss et al. 2000)
  215 (deionized water, batch equilibrium, Ladaa et al. 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2666 (extrapolated, data presented in graph, McGovern 1943)

2397* (Antoine eq. regression, temp range –20.6 to 120.8°C, Stull 1947)

2462 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)

log (P/mmHg) = 7.02003 – 1415.5/(221.0 + t/°C); temp range 34–187°C (Antoine eq. for liquid state, Dreisbach 1959)

2453* (vapor-liquid equilibrium VLE data, measured range 27.887–108°C, Polák et al. 1970)

log (P/mmHg) = 7.05854 – 1438.947/(233.368 + t/°C); temp range 27.887–108°C (ebulliometry, Polák et al. 1970)

4524* (37.088°C, temp range 37.088–119.650°C, Boublik & Aim 1972; quoted, Boublik et al. 1984)

2394 (calculated-Antoine eq., Weast 1972–73)

log (P/mmHg) = [–0.2185 × 9240.5/(T/K)] + 8.026207; temp range –20.6 to 120.8°C (Antoine eq., Weast 1972–73)

2388 (calculated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 6.97183 – 1386.915/(217.526 + t/°C); temp range 37–119°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

1866 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)

640, 1893, 2480 (1.5, 20, 25°C, interpolated from literature data, Dilling 1977)

2417, 2456 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.10343 – 1387.956/(217.64 + t/°C), temp range: 37–120°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.19467 – 1445.722/(224.074 + t/°C), temp range: 26.9–108°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

2465 (Daubert & Danner 1986; quoted, Howard 1990)

2462 (selected, Riddick et al. 1986)

log (P/kPa) = 6.10170 – 1386.90/(217.52 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

2415 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.1017 – 1386.9/(–55.63 + T/K), temp range: 310–393 K, (Antoine eq., Stephenson & Malanowski 1987)

2479, 4319 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

log (P/mmHg) = 30.4038 – 1.5265 × 10^3/(T/K) – 8.783·log (T/K) – 2.6364 × 10^{-9}·(T/K) + 9.4381 × 10^{-6}·$(T/K)^2$; temp range 142–306 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2718 (exptl.-1/K_{AW} = C_W/C_A, Hine & Mookerjee 1975)

248, 581 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)

1621 (20°C, batch stripping-GC, Mackay et al. 1979)

2006 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

log (H/atm) = 10.38 – 2159.0/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)

1635* (equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)

ln (k_H/atm) = 16.05 – 3539/(T/K); temp range 1.0–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

1528 (20°C, gas stripping-GC, Munz & Roberts 1982)

1316 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)

1317; 1175 (20°C, EPICS-GC; gas stripping-GC, measured range 10–30°C, Lincoff & Gossett 1984)

ln [H/(atm m^3/mol)] = 13.12 – 5119/(T/K); temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)

ln [H/(atm m^3/mol)] = 11.32 – 4622/(T/K); temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)

2908 (adsorption isotherm, Urano & Murata 1985)

1445 (20°C, multiple equilibration, Munz & Roberts 1986)

1852* (EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)

ln [H/(atm m^3/mol)] = 12.45 – 4918/(T/K); temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)

1445 (20°C, EPICS-GC, Munz & Roberts 1987)

log K_{AW} = 5.92 – 1802/(T/K); temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

2908 (gas stripping-GC, Warner et al. 1987)
1304 (20°C, EPICS-GC, Yurteri et al. 1987)
1733* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 10.65 – 4368/(T/K); temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)
1363* (tap water, EPICS-GC, temp range 25–47.2°C, Tancréde & Yanagisawa 1990)
log K_{AW} = 7.481 – 2279/(T/K); temp range 25–47.2°C (EPICS-GC, Tancréde & Yanagisawa 1990)
2721 (computed value, Yaws et al. 1991)
1759* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
ln (1/K_{AW}) = –5.13 + 1736/(T/K); temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
1599 (γ^∞ from gas stripping-GC, Li et al. 1993)
1723* (static headspace-GC, temp range 25–45°C, Robbins et al. 1993)
1490* (EPICS-GC/FID, temp range 2–25°C, Dewulf et al. 1995)
717, 1914 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
ln K_{AW} = –4528/(T/K) + 0.01080·Z + 14.655; with Z salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)
1319 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
1200 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)
1710* (equilibrium headspace-GC, temp range 15–45°C, Peng & Wan 1997)
log (k_H/atm) = 9.06 – 1822/(T/K), temp range 15–45°C (headspace-GC measurements, Peng & Wan 1997)
1260 (20°C, headspace equilibrium-GC, Peng & Wan 1998)
2200* (sea water 36‰ NaCl, headspace-GC, temp range 15–45°C, Peng & Wan 1998)
log (k_H/atm) = 9.09 – 1795/(T/K); sea water 36‰ NaCl, temp range 15–45°C (headspace-GC measurements, Peng & Wan 1998)
1159.2 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
2890 (modified EPICS method-GC, Ryu & Park 1999)
1781* (calculated-P/C(exptl. measured), temp range 22–161°C, Knauss et al. 2000)
1690 (static headspace method, Ladaa et al. 2001)
1299 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 6.394 – 1955/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C. Additional data at other temperatures designated * are compiled at the end of this section:

2.60 (shake flask-GC, Chiou et al. 1977)
2.60 (shake flask, Hansch & Leo 1979)
2.53 (shake flask-LSC, Banerjee et al. 1980)
2.53 (shake flask-LSC, Veith et al. 1980,1983; Veith & Kosian 1982)
2.67 (RP-HPLC-RT correlation, Veith et al. 1980)
3.78 (HPLC-RT correlation, McDuffie 1981)
3.30, 2.72–3.57 (shake flask method: mean, range of mean values, OECD 1981)
3.40 (shake flask, Hansch & Leo 1985, 1987)
3.40 (correction of Ball & Roberts 1991 selection, Ball & Roberts 1992)
3.40 (recommended, Sangster 1993)
3.40 (recommended, Hansch et al. 1995)
2.27* (24.8°C, EPICS-GC, measured range 2.2–24.8°C Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

3.48 (head-space GC/FID, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

1.59 (trout, Neely et al. 1974)
1.598 (trout muscle, calculated-ratio of rate const. k_1/k_2, Neely et al. 1974)
1.45–1.88 (calculated-K_{OW}, Veith et al. 1979; Veith et al. 1980)
–1.70 (male Albino rats, Geyer et al. 1980)
1.69 (bluegill sunfish, Barrows et al. 1980)

1.49 (calculated-S, Kenaga 1980)
1.69 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
2.35 (calculated-K_{OW}, Lyman et al. 1982)
2.40 (microorganisms-water, Mabey et al. 1982)
2.06 (rainbow trout, Veith & Kosian 1982)
1.70 (calculated-MCI χ, Koch 1983)
1.70, 2.30 (quoted, calculated, Sabljic 1987)
1.60 (calculated-solvatochromic parameters, Hawker 1990)
2.40 (calculated-K_{OW}, McCarty et al. 1992)
1.79 (rainbow trout, Saito et al. 1992)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

2.38 (calculated, Kenaga & Goring 1980, Kenaga 1980)
2.32 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
2.14; 2.54, 2.89; 2.35, 2.57 (calculated-K_{OW}; calculated-S and mp; calculated-S, Karickhoff 1981)
2.23 (average of 3 sediments and 5 soils, batch equilibrium, Schwarzenbach & Westall 1981)
2.04 (Schwarzenbach & Westall 1981)
3.23 (calculated-K_{OW}, Lyman et al. 1982)
2.38 (peaty soil, calculated-K_{OM}, Friesel et al. 1984)
2.56 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
2.56 (soil, Chiou et al. 1988)
2.00 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.76, 2.53 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.75 (untreated Marlette soil Bt horizon, OC 0.30%, batch equilibrium, Lee et al. 1989)
2.87, 2.78 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.64 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
3.29 (20°C, weathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
4.03 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
2.39, 2.57 (20°C, calculated-K_{OW}, Grathwohl 1990)
2.14 (calculated-molecular conductivity index, Olsen & Davis 1990)
2.45 (2.57% organic carbon in surface soil, Pignatello 1990,1991)
1.81–2.95 (calculated-K_{OW}, Ball & Roberts 1991)
3.60 (Borden organic phase with no mineral sorption, Ball & Roberts 1991)
2.90 (Borden organic phase with no mineral sorption but with Curtis et al. 1986 correlation, Ball & Roberts 1992)
2.62, 2.79, 2.74, 2.80, 2.85, 2.78, 2.83 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon f_{OC} = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)
0.393–1.943 (19 soils from U.S. and China with polar organic carbon POC ranging form 2.89–59.9% and organic carbon OC ranging from 1.08–50.8%, batch sorption equilibrium, Kile et al. 1999)
1.13–2.11 (9 freshwater sediments from U.S. and China with polar organic carbon POC ranging form 5.36–52.5% and organic carbon OC ranging from 0.58–5.62%, batch sorption equilibrium, Kile et al. 1999)
2.32, 2.45, 2.22 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:

1.70 (untreated A horizon Marlette soil, Lee et al. 1989)
2.56, 2.30(A horizon Marlette soil treated with HDTMA, DDTMA, Lee et al. 1989)
1.64 (untreated B_t horizon Marlette soil, Lee et al. 1989)
2.75, 2.64 (treated B_t horizon Marlette soil with HDTMA, DDTMA, Lee et al. 1989)
2.32, 1.90 (quoted, calculated-molecular conductivity index, Olsen & Davis 1990)
3.20; 2.40 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{½}$:

Volatilization: evaporation $t_{½}$(exptl) = (27 ± 3) min for 1 mg/L in water when stirred at 200 rpm at approximately 25°C in an open container of 65 mm deep and $t_{½}$(calc) = 0.56 min (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

Evaporation $t_{½}$(exptl) = 20–27.1 min, $t_{½}$(calc) = 0.20, 26.5 min at 20–25°C, and $t_{½}$(exptl) = 37.5 min, $t_{½}$(calc) = 27 min at .15°C from water (Dilling 1977)

ratio of evaporation rate constant to that of oxygen reaeration: a measured value of 0.44 to that of 0.40 as predicted (Smith et al. 1980);

$t_{½}$ = 5–12 d from pond, $t_{½}$ = 3 h-7 d from river, $t_{½}$ = 3.6–14 d from lake were estimated using representative reaeration rates (Lyman et al. 1982; quoted, Howard 1990);

estimated $t_{½}$ ~ 4.2 h from water (Thomas 1982);

rate constants: k = 0.028 d^{-1}, $t_{½}$ = 25 d in spring at 8–16°C, k = 0.051 d^{-1}, $t_{½}$ = 14 d in summer at 20–22°C, k = 0.056 d^{-1}, $t_{½}$ = 12 d in winter at 3–7°C for the periods when volatilization appears to dominate, and k = 0.057 d^{-1}, $t_{½}$ = 12.1 d with $HgCl_2$, and k = 0.058 d^{-1}, $t_{½}$ = 12.0 d without $HgCl_2$ as poison in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 6.8 ppm/min per gram of catalyst (Ollis 1985); rate constant of 3.09×10^{-3} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O3} < 2 \times 10^{-23}$ cm³ molecule⁻¹ s⁻¹ at 297 K (Mathias et al. 1974; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{OH} = 1.3 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a lifetime about 10 d (Yung et al. 1975; quoted, Callahan et al. 1979)

$k_{OH} = 1.7 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow system-LMR, Howard 1976)

$k_{OH}* = (1.69 \pm 0.07) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 297 K, measured range 297–420 K with calculated lifetime of 0.4–0.6 yr in troposphere (discharge flow system-RF, Chang & Kaufman 1977)

$k_{OH} = (0.13 \pm 0.04) \times 10^{10}$ cm^3 M^{-1} s^{-1} at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1978)

$k_{OH} = 1.70 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson et al. 1979, 1982; quoted, Tuazon et al. 1984; Atkinson et al. 1987)

$k_{OH} = 1.7 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}, residence time of 68 d, loss of 1.5% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{OH} = 1.0 \times 10^{11}$ cm^3 mol^{-1} s^{-1}, and $k_{O3} = 1.0 \times 10^{3}$ cm^3 mol^{-1} s^{-1} at 300 K (estimated, Lyman 1982)

k << 100 M^{-1} h^{-1} for singlet oxygen 25°C (Mabey et al. 1982)

completely degraded in an hour (Dimitriades et al. 1983; quoted, Howard 1990)

k < 0.1 M^{-1} s^{-1} for reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{O3} < 2 \times 10^{-23}$ cm^3 $molecule^{-1}$ s^{-1}, $k_{OH} = 1.7 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Tuazon et al. 1984)

$k_{OH}* = 1.67 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1985)

k_{OH}(calc) = 4.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.7×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{NO3} < 4.0 \times 10^{-17}$ cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{NO3} < 4.0 \times 10^{-17}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated atmospheric lifetime $\tau > 240$ d, $k_{OH} = 1.7 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} with lifetime $\tau = 140$ d, and $k_{O3} < 2 \times 10^{-23}$ cm^3 $molecule^{-1}$ s^{-1} with a lifetime $\tau > 2 \times 10^{3}$ yr at room temp. (Atkinson et al. 1987)

k_{OH}(calc) = 1.8×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.66×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH} = 2.34 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, $k_{NO3} = 9.7 \times 10^{-17}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (Atkinson 1990)

$k_{NO3} < 5.20 \times 10^{-17}$ cm^3 $molecule^{-1}$ s^{-1} relative to ethene at 298 ± 2 K (Atkinson 1991)

Hydrolysis: k = 0.079 $month^{-1}$ at 25°C with $t_{½}$ = 8.8 months (Dilling et al. 1975; quoted, Callahan et al. 1979); abiotic hydrolysis or dehydrohalogenation $t_{½}$ = 8.8 months (Olsen & Davis 1990)

Biodegradation: aqueous aerobic $t_{½}$ = 4320–8640 h, based on aerobic river die-away test data (Mudder 1981; quoted, Howard et al. 1991) and saltwater grab sample test data (Jensen & Rosenberg 1975; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 2352–39672 h, based on anaerobic screening test data (Bouwer et al. 1981; quoted, Howard et al. 1991);

first-order k = 1.1 yr^{-1} with $t_{½}$ = 230 d (Roberts et al. 1982; quoted, Olsen & Davis 1990)

$t_{½}$ = 34 d (Wood et al. 1985; quoted, Olsen & Davis 1990).

$t_{½}$(aerobic) = 180 d, $t_{½}$(anaerobic) = 98 d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant for bacteria k = 1×10^{-10} ml cell^{-1} h^{-1} (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

k_1 = 3.323 h^{-1}; k_2 = 0.0823 h^{-1} (trout muscle, Neely et al. 1974)

k_1 = 11.4 h^{-1} (flagfish, calculated-BCF × k_1, McCarty et al. 1992)

k_2 = 0.0454 h^{-1} (flagfish, estimated-one compartment first-order kinetic, McCarty et al. 1992)

k_1 = 3.30 h^{-1}; k_2 = 0.0833 h^{-1} (trout, Hawker & Connell 1985)

Half-Lives in the Environment:

Air: tropospheric $t_{½}$ = 12 wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{½}$ > 10 d for the reaction with OH radical (Darnall et al. 1976);

lifetime ~ 10 d, based on reaction with OH radical (Yung et al. 1975; quoted, Callahan et al. 1979);

photodecomposition $t_{½}$ = 14.2 h with NO and $t_{½}$ = 8.3 h with NO_2 under simulated atmospheric conditions (Dilling et al. 1976);

estimated N. troposphere residence time of 150 d by one compartment nonsteady state model (Singh et al. 1978);

lifetime of 1.0 yr in troposphere (Altshuller 1980);

residence time of 68 d, loss of 1.5% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

estimated troposphere residence time of 200–390 d (Lyman 1982);

$t_{½}$ = 384–3843 h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetimes: τ > 240 d for the reaction with NO_3 for a 12-h nighttime average concentration of 2.4×10^9 molecule/cm^3, τ = 140 d for the reaction with OH radical for a 12-h average concentration of 1.0×10^6 molecule/cm^3, and τ > 2000 yr for the reaction with O_3 for a 24-h average concentration of 7×10^{11} molecule/cm^3 (Atkinson et al. 1987).

Surface water: estimated $t_{½}$ = 9.9–32 d in surface waters at various locations in case of a first order reduction process; $t_{½}$ = 3–30 d in rivers, $t_{½}$ = 30–300 d in lakes and ground waters (Zoeteman et al. 1980)

$t_{½}$ = 25 d in spring at 8–16°C, 14 d in summer at 20–22°C and 12 d in winter at 3–7°C when volatilization dominates, and $t_{½}$ = 12.1 d and 12.0 d for experiments with and without $HgCl_2$ as poison respectively in September 9–15 in marine mesocosm (Wakeham et al. 1983)

$t_{½}$ = 4320–8640 h, based on aerobic river die-away test data (Mudder 1981; quoted, Howard et al. 1991) and saltwater sample grab data (Jensen & Rosenberg 1975; quoted, Howard et al. 1991);

calculated $t_{½}$ = 10 d and 32 d concentration reduction between sampling points on the Rhine River and a lake in the Rhine basin, respectively (Zoeteman et al. 1980; quoted, Howard 1990)

$t_{½}$(aerobic) = 180 d, $t_{½}$(anaerobic) = 98 d in natural waters (Capel & Larson 1995).

Ground water: $t_{½}$ = 8640–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ < 10 d (Ryan et al. 1988);

$t_{½}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{½}$ < 1 d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{½}$ = 14 h, clearance from fish in simulated ecosystem (Neely 1980);

$t_{½}$ < 10 d, subject to plant uptake via volatilization (Ryan et al. 1988);

$t_{½}$ = 0.4–0.5 d to eliminate from lsmall fish (McCarty et al. 1992).

TABLE 5.1.1.31.1
Reported aqueous solubilities of tetrachloroethylene at various temperatures

$$S/(wt\%) = 1.49696 \times 10^{-2} - 7.8009 \times 10^{-6}\cdot(t/°C) - 5.1403 \times 10^{-7}\cdot(t/°C)^2 + 3.6938 \times 10^{-8}\cdot(t/°C)^3 \qquad (1)$$

$$S/(wt\%) = 0.26479 - 1.5487 \times 10^{-3}\cdot(T/K) + 2.4477 \times 10^{-6}\cdot(T/K)^2 \qquad (2)$$

Horvath 1982		**Stephenson 1992**		**Horvath & Getzen 1999a**		**Knauss et al. 2000**	
summary of literature data		**shake flask-GC**		**summary of literature data**		**batch equilibrium-GC**	
t/°C	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**
						at 1.0 MPa	
0	149.7	0	273	0	244	23	192.3
10	148.8	9.5	270	5	234	51	247.4
20	149	19.5	286	10	224	75	313.8
25	150.3	31.1	221	15	218	101	519
30	152.7	40.0	213	20	211	124	1006
40	162	50.1	273	25	206	150	1895
50	179.1	61.3	304	30	202	161	2513
60	206.3	71	377	35	200		
70	245.7	80.2	380	40	198		
80	299.7	91.8	523	45	198		
				50	199		
eq. 1	S/wt%			55	202		
				60	205		
				65	210		
				70	216		
				eq. 2	S/wt%		
				temp range 273–343 K			

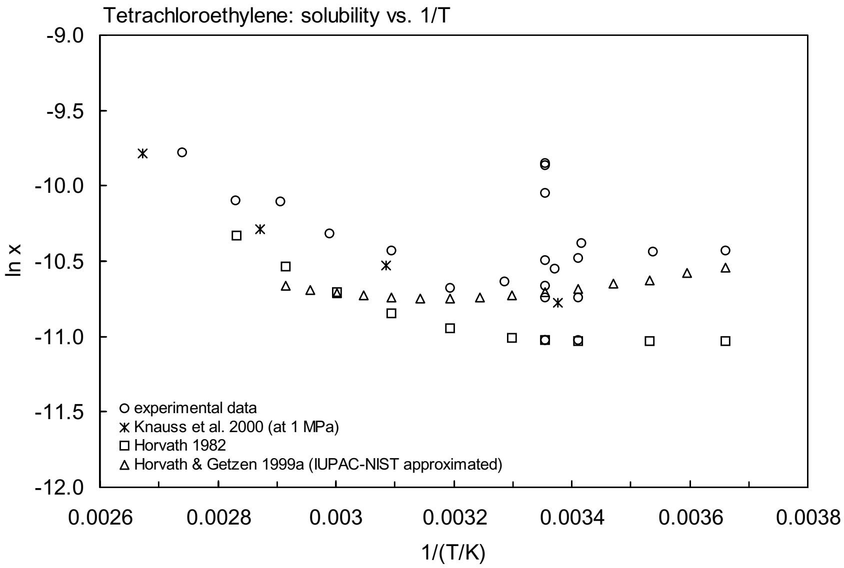


FIGURE 5.1.1.31.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.2
Reported vapor pressures of tetrachloroethylene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		**Polak et al. 1970**		**Boublik & Aim 1972**	
summary of literature data		**vapor-liquid equilibrium**		**in Boublik et al. 1984**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
–20.6	133.3	27.887	2869	37.088	4524
2.40	666.6	35.758	4274	46.239	6967
13.8	1333	41.702	5689	52.671	9306
26.3	2666	46.502	7101	58.697	12046
40.1	5333	57.065	11276	63.270	14549
49.2	7999	61.254	15412	68.545	17921
61.3	13332	68.065	17620	73.064	21314
79.8	26664	74.529	22541	78.165	25780
100.0	53329	81.957	29555	82.292	29923
120.8	101325	88.055	36557	87.183	35493
		94.568	45465	91.791	41470
mp/°C	–19.0	98.917	52316	97.291	49704
		104.269	61875	103.930	61295
		107.692	68694	111.548	77125
				119.650	97337
				eq. 2	P/kPa
				A	6.10343
				B	1387.956
				C	217.640
				bp	121.074

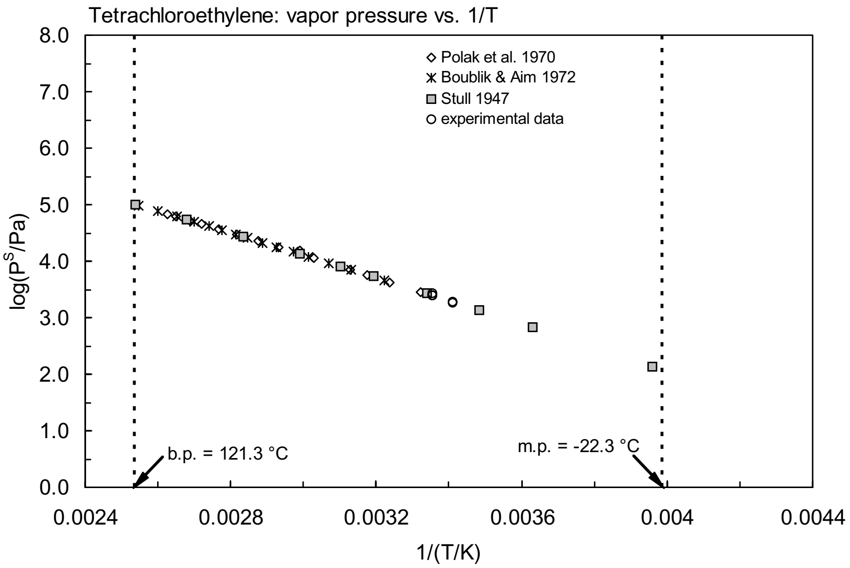


FIGURE 5.1.1.31.2 Logarithm of vapor pressure versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.3
Reported Henry's law constants of tetrachloroethylene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2)
$\ln (k_H/atm) = A - B/(T/K)$ (3)
$\ln [H/(Pa\ m^3/mol)] = A - B/(T/K)$ (4)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

$\log K_{AW} = A - B/(T/K)$ (1a)
$\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\log (k_H/atm) = A - B/(T/K$ (3a)
$\ln [H/(atm\cdot m^3/mol)] = A - B/(T/K)$ (4a)

1.

Leighton & Calo 1981		**Gossett 1987**		**Tancréde & Yanagisawa 1990**		**Kolb et al. 1992**	
equilibrium cell-GC		**EPICS-GC**		**EPICS-GC**		**equilibrium headspace-GC**	
t/°C	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**
1.0	377.4	9.6	691	25	1363	40	1759
1.0	413.5	17.5	1186	26.5	1694	60	2080
1.2	430.6	24.8	1793	27.4	2224	70	3658
2.5	474.9	34.6	2857	28.9	2160	80	3375
7.0	572.9			28.9	2034		
10.0	675.2			29.7	2770	eq. 2	$1/K_{AW}$
12.0	731.4	eq. 4	H/(atm m³/mol)	29.9	2998	A	–5.13
12.0	797.6	A	12.45	33.3	3057	B	–1736
12.9	826.0	B	4918	35.6	2413		
14.0	914.7			38.3	2745		
18.0	1122			40	4895		
18.0	1144	**Ashworth et al. 1988**		44.7	5549		
18.0	1145	**EPICS-GC**		45	6004		
19.0	1176	**t/°C**	**H/(Pa m³/mol)**	47.2	5886		
19.2	1156						
19.5	1182	10	857.2	eq. 1a	K_{AW}		

TABLE 5.1.1.31.3 *(Continued)*

Leighton & Calo 1981		Gossett 1987		Tancréde & Yanagisawa 1990		Kolb et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		equilibrium headspace-GC	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
24.3	1583	15	1125	A	7.481		
25.2	1623	20	1429	B	2279		
25.3	1651	25	1733				
26.0	1636	30	2482				
26.0	1712						
26.1	1679	eq. 4	H/(atm m^3/mol)				
		A	10.65				
eq. 3	k_H/atm	B	4368				
A	22.68						
B	4735						

2.

Robbins et al. 1993		Dewulf et al. 1995		Peng & Wan 1997		Knauss et al. 2000	
headspace-GC		EPICS-GC		equilibrium headspace-GC		calculated-P/C	
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
25	1723	2.0	359.2	15	1016	22	1781
30	2340	6.0	2492	20	1272	51	5837
40	3070	10.0	602.7	25	1710	75	10328
45	2847	18.2	995.6	30	2160	101	18540
		25.0	1490	35	2713	124	19157
				40	3283	150	20200
		eq. 1	K_{AW}	45	4108	161	19844
		A	14.655				
		B	4528	eq. 3a	k_H/atm		
				A	9.06		
				B	1822		

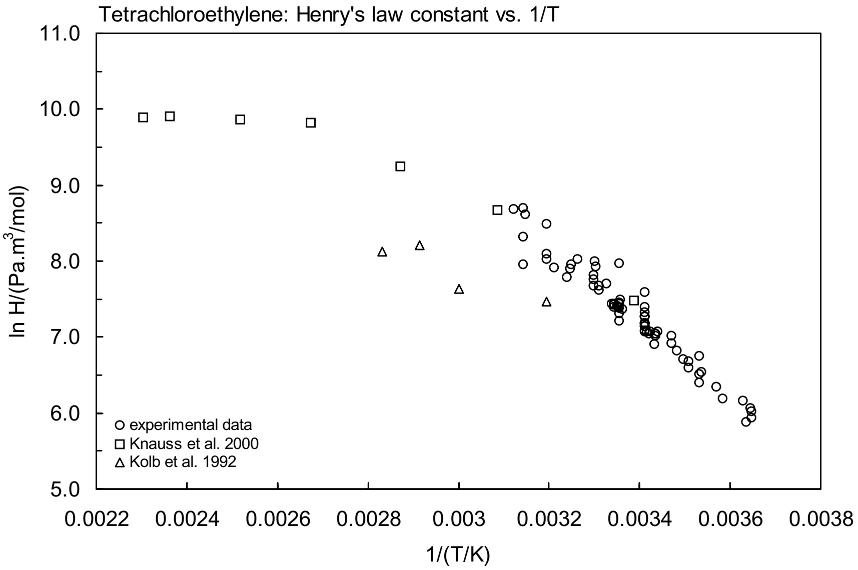


FIGURE 5.1.1.31.3 Logarithm of Henry's law constant versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.4
Reported octanol-water partition coefficients of tetrachloroethylene at various temperatures

Dewulf et al. 1999	
EPICS-GC	
t/°C	log K_{OW}
2.2	2.25
6.0	2.27
10.0	2.38
14.1	2.32
18.7	2.36
24.8	2.27

change in enthalpy:
$\Delta H_{OW}/(\text{kJ mol}^{-1}) = 2.6$
(–11.1 to 16.3)
enthalpy of transfer
$\Delta H_{oct}/(\text{kJ mol}^{-1}) = 4.7$
(–9.0 to 18.4)

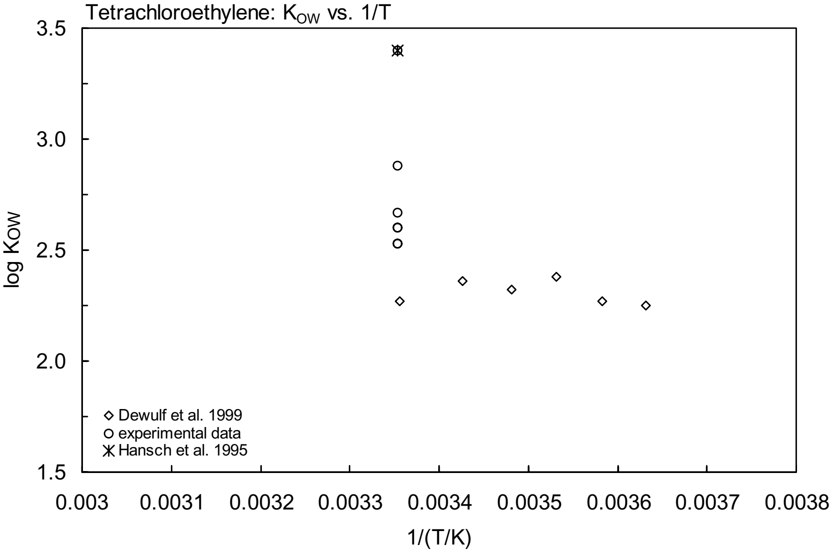
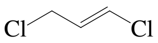


FIGURE 5.1.1.31.4 Logarithm of K_{OW} versus reciprocal temperature for tetrachloroethylene.

5.1.1.32 1,3-Dichloropropene



Common Name: 1,3-Dichloropropene
Synonym: 1,3-dichloropropylene, 1,3-dichloro-1-propene, Telone II
Chemical Name: 1,3-dichloropropene
CAS Registry No: 542-75-6
Molecular Formula: $C_3H_4Cl_2$, $CH_2ClCH=CHCl$
Molecular Weight: 110.970
Melting Point (°C):
Boiling Point (°C):
  112.0 (*trans*-stereoisomer I, Horvath 1982; McNally & Grob 1984; Dean 1985; Lide 2003)
  104.3 (*cis*-stereoisomer II, Horvath 1982; McNally & Grob 1984; Dean 1985: Lide 2003)
Density (g/cm^3 at 20°C):
  1.224 (*trans*-stereoisomer I, Horvath 1982; McNally & Grob 1984)
  1.217 (*cis*-stereoisomer II, Horvath 1982; McNally & Grob 1984)
Molar Volume (cm^3/mol):
  91.2 (*trans*-stereoisomer I, 20°C, calculated-density)
  90.7 (*cis*-stereoisomer II, 20°C, calculated from density)
  108.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  2800 (*trans*-stereoisomer I, Dilling 1977)
  2700 (*cis*-stereoisomer II, Dilling 1977)
  2723 (recommended, Horvath 1982)
  1071 (*trans*-stereoisomer I, headspace-GC, McNally & Grob 1983)
  1088 (*cis*-stereoisomer II, headspace-GC, McNally & Grob 1983)
  1020 (30°C, *trans*-stereoisomer I, headspace-GC, McNally & Grob 1984)
  911 (30°C, *cis*-stereoisomer II, headspace-GC, McNally & Grob 1984)
  1000 (20°C, Wauchope et al. 1992)
  2250 (Wauchope et al. 1992)
  4533, 4311, 4223 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated):
  4533, 5733 (*trans*-, *cis*-stereoisomer, data from Dow Chemicals, Dilling 1977)
  435, 569 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
  3333 (20°C, selected, Mills et al. 1982)
  3334 (20°C, quoted, Warner et al. 1987)
  3866 (20°C, Wauchope et al. 1992)

Henry's Law Constant (Pa m^3/mol at 25°Cor as indicated):
  232 (calculated-P/C, Dilling 1977)
  137 (calculated-P/C, Warner et al. 1987)
  122, 198, 302 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)

Octanol/Water Partition Coefficient, log K_{OW}:
  1.98 (selected, Mills et al. 1982)
  1.41 (quoted, Verhaar et al. 1992)
  1.84 (*cis/trans*, calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.505 (soil, selected, Wauchope et al. 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 31 min in water from stirring in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975)

$t_{½}$(exptl) = 29.6 min, $t_{½}$(calc) = : 2.4 min, 23.8 min for *cis*-stereoisomer, and $t_{½}$(calc) = : 3.2 min, 24.6 min for *trans*-stereoisomer from water (Dilling 1977)

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (7.74 \pm 0.2) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} *cis*-isomer, $k_{OH} = (1.31 \pm 0.05) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for *trans*-isomer at 22 ± 2°C, calculated $t_{½}$ = 12 h and 7 h for the *cis*- and *trans*-isomer, respectively (relative rate method, Tuazon et al. 1984)

$k_{O3} = 1.5 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} *cis*-isomer, $k_{O3} = 6.7 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} for *trans*-isomer at room temp., calculated $t_{½}$ = 52 d and 12 d for *cis*- and *trans*-isomer, respectively (relative rate method, Tuazon et al. 1984)

k_{OH}(calc) = 1.1×10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 7.5×10^{-12} cm^3 molecule^{-1} s^{-1} for *cis*-isomer; k_{OH}(calc) = 1.3×10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 1.26×10^{-11} cm^3 molecule^{-1} s^{-1} for *trans*-isomer at room temp. (SAR [structure-activity relationship], Atkinson 1985)

k_{OH}(calc) = 8.8×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 8.45×10^{-12} cm^3 molecule^{-1} s^{-1} for *cis*-isomer; k_{OH}(calc) = 10.0×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 14.4×10^{-12} cm^3 molecule^{-1} s^{-1} for *trans*-isomer at room temp. (SAR [structure-activity relationship], Atkinson 1987)

Hydrolysis: $t_{½}$ = 133–271 h, based on measured rate constants for hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991);

rate of hydrolysis is, however, independent of pH over the range of pH 5 to pH 10 (McCall 1987).

Biodegradation: aqueous aerobic $t_{½}$ = 168–672 h, based on unacclimated aqueous aerobic biodegradation screening studies (Tabak et al. 1981; Krijgheld & Van der Gen 1986; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 672–2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 0.24–2.4 h from air for the reaction with OH radicals (Darnall et al. 1976);

$t_{½}$(calc) = 12 h and 7 h for the *cis*- and *trans*-isomer, respectively, for reactions with OH radical; $t_{½}$(calc) = 52 d and 12 d for *cis*- and *trans*-isomer, respectively, for reactions with O_3 at room temp. (Tuazon et al. 1984).

$t_{½}$ = 4.66–80.3 h, based on measured rate constants for reaction with OH radical and ozone (Howard et al. 1991)

Surface water: $t_{½}$ = 133–271 h, based on measured rate of hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991).

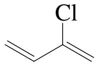
Ground water: $t_{½}$ = 133–271 h, based on measured rate of hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 133–271 h, based on measured rate of hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991).

Biota:

5.1.1.33 Chloroprene



Common Name: Chloroprene
Synonym: 2-chloro-1,3-butadiene
Chemical Name: 2-chloro-1,3-butadiene
CAS Registry No: 126-99-8
Molecular Formula: C_4H_5Cl, $CH_2{=}CClCH{=}CH_2$
Molecular Weight: 88.536
Melting Point (°C):
  –130 (Kirk-Othmer 1985; Verschueren 1983; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
  59.4 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)
  69.145 (Boublik et al. 1984)
Density (g/cm^3 at 20°C):
  0.9583 (Weast 1982–83; Dean 1985)
  0.9580 (Verschueren 1983)
Molar Volume (cm^3/mol):
  92.4 (20°C, calculated-density, Stephenson & Malanowski 1987)
  102.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  964000 (20°C, saturation concentration, Verschueren 1983)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  26660, 36660 (20°C, 30°C, Verschueren 1983)
  28740 (interpolated-Antoine eq., Boublik et al. 1984)
  $\log (P/kPa) = 5.30955 - 793.85/(181.137 + t/°C)$, temp range: 20–60°C (Antoine eq. from reported exptl. data Boublik et al. 1984)
  28780 (interpolated-Antoine eq., Dean 1985, 1992)
  $\log (P/mmHg) = 6.16150 - 783.45/(197.7 + t/°C)$; temp range 20–60°C (Antoine eq., Dean 1985, 1992)
  29450 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
  $\log (P_L/kPa) = 6.652 - 1545.3/(T/K)$; temp range: 279–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  $\log (P_L/kPa) = 6.6519 - 1545.0/(T/K)$; temp range 243–263 K (Antoine eq.-II, Stephenson & Malanowski 1987)
  23200 (quoted, Howard 1989)
  $\log (P/mmHg) = 8.9353 - 1.9176 \times 10^3/(T/K) + 0.73836 \cdot \log (T/K) - 8.4743 \times 10^{-3} \cdot (T/K) + 6.0224 \times 10^{-6} \cdot (T/K)^2$; temp range 143–525 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
  3242 (estimated by bond contribution method, Howard 1989)

Octanol/Water Partition Coefficient, log K_{OW}:
  2.03 (Howard 1989)

Bioconcentration Factor, log BCF:
  1.342 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:
  2.498 (soil, estimated-K_{OW}, Lyman et al. 1982)

1.699 (soil, molecular topology and QSAR, Sabljic 1984)

Environmental Fate Rate Constants, k and Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ ~ 3 h from a model river 1 m deep with a current velocity of 1 m/s and a wind speed of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{½}$ = 2.9–27.8 h, based on estimated rate constants for the reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{½}$ = 672–4320 h, based on aqueous aerobic screening test data for vinyl chloride (Helfgott et al. 1977; Freitag et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 0.24–2.4 h from air for the reaction with OH radicals (Darnall et al. 1976);

$t_{½}$ = 1.8 h for the reaction with photochemically produced hydroxyl radicals and $t_{½}$ = 12 h for the reaction with ozone in atmosphere (Cupitt 1980; quoted, Howard 1989);

$t_{½}$ = 2.9–27.8 h, based on estimated rate constants for reaction with hydroxyl radicals and ozone in air (Atkinson & Carter 1984; Atkinson 1987; quoted, Howard et al. 1991).

Surface water: estimated $t_{½}$ = 6.7–53 d in surface waters at various locations in case of a first order reduction process; and $t_{½}$ = 3–30 d in rivers, $t_{½}$ = 30–300 d in lakes and ground waters (Zoeteman et al. 1980)

$t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

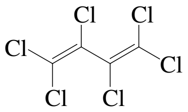
Ground water: $t_{½}$ = 1344–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

5.1.1.34 Hexachlorobutadiene



Common Name: Hexachlorobutadiene
Synonym: HCBD, perchloro-1,3-butadiene
Chemical Name: 1,1,2,3,4,4-hexachloro-1,3-butadiene
CAS Registry No: 87-68-3
Molecular Formula: C_4Cl_6, $Cl_2C{=}CClClC{=}CCl_2$
Molecular Weight: 260.761
Melting Point (°C):
  -21.0 (Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
  215 (Horvath 1982; Lide 2003)
Density (g/cm^3 at 20°C):
  1.682 (Horvath 1982)
Molar Volume (cm^3/mol):
  155.2 (20°C, calculated-density, Stephenson & Malanowski 1987)
  206.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  0.20 (Melnikov 1971)
  2.00 (20°C, Pearson & McConnell 1975)
  3.23 (shake flask-HPLC, Banerjee et al. 1980)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  20.0 (20°C, Pearson & McConnell 1975)
  $\log (P/kPa) = 6.06503 - 1520.873/(163.685 + t/°C)$; temp range 70–200°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
  $\log (P_L/kPa) = 6.4781 - 1783.8/(-84.48 + T/K)$; temp range 343–484 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
  2604 (calculated-P/C, Warner et al. 1987)
  1044 (batch stripping, Warner et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
  4.74 (HPLC-RT correlation, Konemann et al. 1979)
  4.78 (shake flask-HPLC, Banerjee et al. 1980)
  4.63 (calculated-fragment const., Könemann 1981)
  4.90 (shake flask-GC, both phases, Chiou 1985)
  4.78 (recommended, Sangster 1993)
  4.78 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
  4.70 (Thomann 1989)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{½}$ = 2965–28650 h, based on an estimated rate constant for vapor phase reaction with OH radicals (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: no hydrolyzable groups, rate constant at pH 7 is zero (Kollig et al. 1987).

Biodegradation: aqueous aerobic $t_{½}$ = 672–4320 h, based on monitoring data and acclimated aqueous screen test data (Howard et al. 1991); aqueous anaerobic $t_{½}$ = 2688–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{½}$ ~ 1.0 wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

$t_{½}$ = 2865–28650 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{½}$ = 672–4320 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

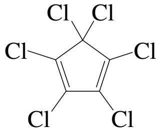
Ground water: $t_{½}$ = 1344–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 672–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

5.1.1.35 Hexachlorocyclopentadiene



Common Name: Hexachlorocyclopentadiene
Synonym: 1,2,3,4,5,5-hexachlorocyclopentadiene, perchlorocyclopentadiene, HCCPD
Chemical Name: 1,2,3,4,5,5-hexachloro-1,3-cyclopentadiene
CAS Registry No: 77-47-4
Molecular Formula: C_5Cl_6
Molecular Weight: 272.772
Melting Point (°C):
–9 (Lide 2003)
Boiling Point (°C):
239 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 20°C): 1.702
Molar Volume (cm^3/mol):
160.3 (20°C, calculated-density, Stephenson & Malanowski 1987)
210.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
0.805 (Shake flask-LSC Lu et al. 1974)
1.80 (Zepp et al. 1979)
0.805 (Callahan et al. 1979; Dobbs et al. 1980; Geyer et al. 1981; Warner et al. 1987; Isnard & Lambert 1988)
1.80 (28°C, vapor saturation or shake flask-GC, Wolfe et al. 1982)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
10.84 (Verschueren 1977; Warner et al. 1987)
10.67 (Wolfe et al. 1982)
11.90 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 7.4813 - 2804.32/(T/K)$; temp range 335–512 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = -9.7942 - 3.3161 \times 10^3/(T/K) + 10.171 \cdot \log (T/K) - 2.1115 \times 10^{-2} \cdot (T/K) + 9.2045 \times 10^{-6} \cdot (T/K)^2$; temp range 284–746 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol):
2736 (concentration ratio-GC, Wolfe et al. 1982)
1662 (batch stripping; Warner et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
5.04 (HPLC-RT correlation, McDuffie 1981)
5.04 (28°C, concentration ratio-GC, Wolfe et al. 1982)
5.26 (HPLC-RT correlation, Eadsforth 1986)
5.04 (recommended, Sangster 1993)
5.04 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.53, 2.97, 3.21, 2.65 (algae, snail, mosquito, fish, Lu et al. 1975)
1.47 (fathead minnow, Veith et al. 1979)
3.04, 3.21 (*Chlorella*, calculated-solubility, Geyer et al. 1981)

1.47, 4.19 (quoted, calculated-K_{OW}, Mackay 1982)
3.18, 3.89 (estimated-S and K_{OW}, Isnard & Lambert 1988)

Sorption Partition Coefficient, log K_{OC}:
4.08 (sediment organic carbon, calculated-K_{OW}, Wolfe et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: appears to be important in flowing waters (Callahan et al. 1979).

Photolysis: near-surface photolysis is an important process with a rate constant $k = 4.9\ d^{-1}$ with $t_{1/2} = 11$ min (Callahan et al. 1979);

direct photolysis in natural waters in midday sunlight of Athens, Georgia at latitude 34°N and 83°W with $t_{1/2} < 10$ min, and near-surface photolysis rate constant k(calc) = $3.9\ h^{-1}$ on cloudless days averaged over both light and dark periods for a year (Wolfe et al. 1982);

photolysis $t_{1/2} = 1.0$ min to 10.7 min, based on photolysis studies in aqueous solutions (Butz et al. 1982; Wolfe et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 1.0$ to 8.9 h, based on calculated rate constants for the vapor phase reactions with OH radicals and O_3 in air (Cupitt 1980; quoted, Howard et al. 1991).

Hydrolysis: appears to be an important fate process with a rate constant $k = 5.6 \times 10^{-7}\ s^{-1}$ at 25°C with $t_{1/2} = 14$ d (Callahan et al. 1979);

reaction rate constant was independent of pH range of about 3 to 10 under most environmental conditions and an extrapolated rate constant $l = 4 \times 10^{-3}\ s^{-1}$ was found at 25°C with $t_{1/2} = 173$ h (Wolfe et al. 1982; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 168$ to 672 h, based on aerobic aqueous screening test data (Tabak et al. 1981; Freitag et al. 1982; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ to 2688 h, based on aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 1.0$ to 8.9 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 1.0$ min to 173 h, based on photolysis and hydrolysis half-lives (Howard et al. 1991); measured rate constant $k = (90 \pm 40)\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 2 and 25 ± 2°C, with $t_{1/2} = 6$ min at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 173$ to 1344 h, based on aerobic aqueous biodegradation and hydrolysis half-lives (Howard et al. 1991).

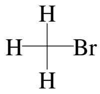
Sediment: hydrolysis rate constant in the sediment was assumed to be the same as that of water and decay rate constant $k = 1.5$ to $5.4 \times 10^{-5}\ s^{-1}$ for natural pond sediment-water system (Wolfe et al. 1982).

Soil: $t_{1/2} = 168$ to 672 h, based on aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biota:

5.1.2 BROMOALKANES AND BROMOALKENES

5.1.2.1 Bromomethane



Common Name: Methyl bromide
Synonym: bromomethane, monobromomethane, Embafume, Terabol
Chemical Name: bromomethane, methyl bromide
CAS Registry No: 74-83-9
Molecular Formula: CH_3Br
Molecular Weight: 94.939
Melting Point (°C):
–93.68 (Lide 2003)
Boiling Point (°C):
3.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.6755, 1.6617 (20°C, 25°C, Dreisbach 1961)
Molar Volume (cm^3/mol):
56.7 (20°C, calculated-density)
52.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
23.26, 24.098 (25°C, at bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
13410* (vapor saturation-gravitational method, measured range 10–32°C, Haight 1951)
20700, 24140 (20°C, 25°C, gravitational method, Glew & Moelwyn-Hughes 1953)
14400 (Irmann 1965; Hine & Mookerjee 1975)
13400 (Jolles 1966; Günther et al. 1968)
12930 (Korenman et al. 1971)
900 (20°C, Verschueren 1977,1983)
15223* (summary of literature data, temp range 5–80°C, Horvath 1982)
17500 (20°C, Windholz et al. 1983)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
256550 (interpolated-Antoine eq. regression, temp range –96.3 to 3.6°C, Stull 1947)
217700 (calculated-Antoine eq., Dreisbach 1959, 1961)
log (P/mmHg) = 6.95965 – 986.59/(238.32 + t/°C); temp range –58 to 53°C (Antoine eq. for liquid state, Dreisbach 1959, 1961)
log (P/mmHg) = 6.95965 – 986.590/(238.32 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
183900 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 5925.9/(T/K)] + 7.482362; temp range –96.3 to 190°C (Antoine eq., Weast 1972–73)
218930 (calculated-Antoine eq., Kudchadker et al. 1979)
log (P/mmHg) = 7.08823 – 1044.42/(244.684 + t/°C) (Antoine eq., Kudchadker et al. 1979)
187000 (20°C, Thomas 1982)
216900, 219000 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.20369 – 1041.723/(244.36 + t/°C); temp range –69.9 to 4.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.2243 – 1049.898/(245.319 + t/°C); temp range –70 to 3.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.21313 – 1044.42/(224.684 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
217680 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.08455 – 986.59/(–34.83 + T/K); temp range 201–296 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 29.3988 – 2.0406 × 10^3/(T/K) –7.9966·log (T/K) – 4.1899 × 10^{-10}·(T/K) + 5.0174 × 10^{-6}·$(T/K)^2$; temp range 179–467 K (vapor pressure eq., Yaws 1994)
218630 (selected and summary of literature data, temp range 179.48–318.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
631*; 621 (exptl.-concn ratio, measured range 5–80°C; calculated-P/C, Glew & Moelwyn-Hughes 1953)
log {H/(mmHg·L/mol)} = 73.022 – 22.261·log (T/K) – 4254.8/(T/K); temp range 278.16–253.16 K (Glew & Moelwyn-Hughes 1953)
733* (29.43°C, concentration ratio, measured range 29.44–49.59°C, Swain & Thornton 1962)
652 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
533 (20°C, calculated-P/C, Mackay & Shiu 1981)
19958 (20°C, calculated-P/C, Mabey et al. 1982)
1317 (calculated-P/C, Thomas 1982)
20260 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
10690 (calculated-P/C, Mackay & Shiu 1990)
687.4 (computed value, Yaws et al. 1991)
204, 515 (0, 22°C, distilled water, headspace-GC, Elliott & Rowland 1993)
596* (gas-liquid equilibrator-GC, measured range 1.1–30.5°C, De Bruyn & Saltzman 1997)
490 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 3.468 – 1221/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
1.19 (shake flask-GC, Leo et al. 1975)
1.19 (Hansch & Leo 1979; Hansch & Leo 1985)
1.19 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, log K_{OA}:
2.11 (calculated-infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
0.623 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
0.672 (calculated-K_{OW}, Lyman et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
2.236, 2.241, 2.215 (Naaldwijk loamy sand, Aalsmeer loam, Boskoop peaty clay, Howard 1989)
0.771 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
2.10 (calculated-S, Lyman et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization: estimated experimental $t_{1/2}$ = 27 min 1 mg/L when stirred at 200 rpm in water at approximately 25°C in an open container (Dilling et al. 1975; quoted, Callahan et al. 1979);
$t_{1/2}$ ~ 30 min (Mills et al. 1982);
$t_{1/2}$ = 3.0 h in a model river (estimated, Lyman et al. 1982; quoted, Howard 1989);
$t_{1/2}$ ~ 0.2 and 0.5 d for the volatilization from 1 and 10 cm of soil, respectively (Jury et al. 1984; quoted, Howard 1989).
Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}* = (4.14 ± 0.43) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 245–375 K with lifetime of 1.32 yr in the troposphere (flash photolysis-RF, Davis et al. 1976)

k_{OH} = 3.5 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow system, Howard & Evenson 1976)

k_{OH} = 4.0 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1}, residence time of 289 d, loss of 0.4% in one day or 12 sunlit hour at 300 K (Singh et al. 1981)

k_{OH} = 2.4 × 10^{10} cm^3 mol^{-1} s^{-1} at 300 K (estimated, Lyman 1982)

k_{OH}* = 3.93 × 10^{-14} cm^3·$molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

k << 360 M^{-1} h^{-1} for singlet oxygen and k = 0.1 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation $t_{½}$ = 1633–16327 h in air, based on measured rates for reaction with OH radicals in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis: first-order k = 4.0 × 10^{-7} s^{-1} with a maximum $t_{½}$ = 20 d at pH 7 and 25°C (Radding et al. 1977; Mabey & Mill 1978; quoted, Callahan et al. 1979);

k = 4.09 × 10^{-7} s^{-1} with $t_{½}$ = 20 d at pH 7 and 25°C (Mabey & Mill 1978)

$t_{½}$ = 470–912 h, based on measured first-order hydrolysis rate constants (Mabey & Mill 1978; Ehrenberg et al. 1974; quoted, Vogel & Reinhard 1986; Howard 1989; Howard et al. 1991);

k = 1.44 × 10^{-3} h^{-1} at pH 7 and 25°C (Callahan et al. 1979; quoted, Mabey et al. 1982)

k = 3 × 10^{-7} s^{-1} at 25°C with $t_{½}$ = 26.7 d (Castro & Belser 1981; quoted, Howard 1989).

Biodegradation: aerobic $t_{½}$(aq.) = 168–672 h, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991);

anaerobic $t_{½}$(aq.) = 672–2688 h, based on unacclimated aqueous aerobic biodegradation half-life (Tabak et al. 1981; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

lifetime of 3.8 yr in the troposphere (Altshuller 1980);

$t_{½}$ = 0.29 y in the atmosphere for the reaction with 2 × 10^6 OH radicals/cm^3 at 25°C (Dilling 1982; quoted, Howard 1989);

$t_{½}$ = 289 d estimated as toxic chemical residence time with rate constant of 4 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} for the reaction with OH radicals at 300 K (Singh et al. 1980,1981; quoted, Howard 1989);

$t_{½}$ = 1633–16327 h, based on measured rates for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 20 d at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{½}$ = 168–672 h, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{½}$ = 336–912 h, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic waste water inoculum and hydrolysis half-life (Tabak et al. 1981; Mabey & Mill 1978; Ehrenberg et al. 1974; quoted, Vogel & Reinhard 1986; Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 168–672 h, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.2.1.1
Reported aqueous solubilities of bromomethane at various temperatures

$$S/(\text{wt\%}) = 1.4019 - 6.3562 \times 10^{-2}\cdot(t/°C) + 1.71977 \times 10^{-3}\cdot(t/°C)^2 - 2.8262 \times 10^{-5}\cdot(t/°C)^3 + 2.5268 \times 10^{-7}\cdot(t/°C)^4 - 9.3470 \times 10^{-10}\cdot(t/°C)^5 \quad (1)$$

Haight 1951		Horvath 1982	
gravitational method		summary of literature data	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
10	26790	5	35000
17	18300	10	27997
25	13410	20	18401
32	11490	25	15223
		30	12804
		40	9517
		50	7430
		60	5919
		70	4757
		eq. 1	S/wt%

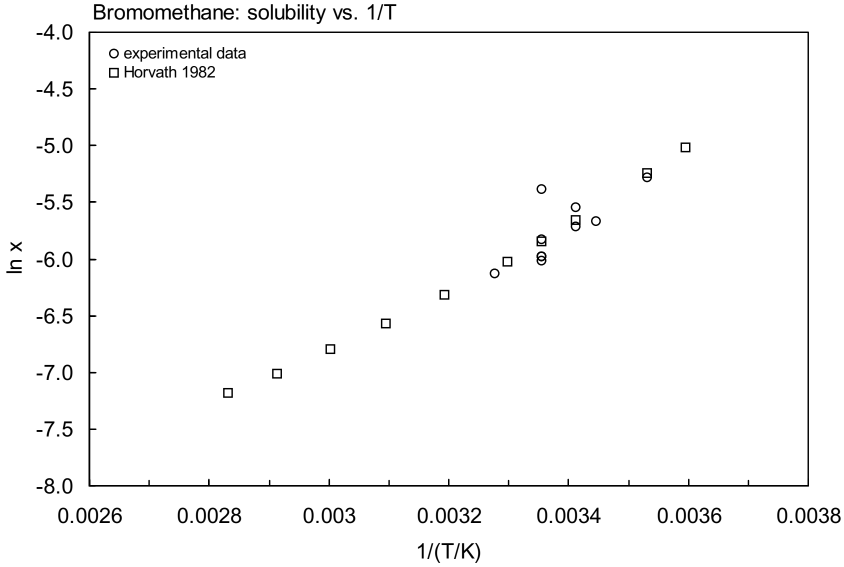


FIGURE 5.1.2.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for bromomethane.

TABLE 5.1.2.1.2

Reported Henry's law constants of bromomethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1)

$\ln (1/K_{AW}) = A - B/(T/K)$ (2)

$\ln (k_H/atm) = A - B/(T/K)$ (3)

$\ln H = A - B/(T/K)$ (4)

$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

$\log H = A - B\cdot\log (T/K) - C/(T/K)$ (6)

$\log K_{AW} = A - B/(T/K)$ (1a)

$\log (1/K_{AW}) = A - B/(T/K)$ (2a)

Glew & Moelwyn-Hughes 1953		**Swain & Thornton 1962**		**De Bruyn & Saltzman 1997**			
concentration ratio		**concentration ratio**		**gas-liquid membrane equilibrator-GC**			
t/°C	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**		
					pure water	seawater	35‰ NaCl
5.0	276	29.43	729	1.1	205.5	253.9	255.2
10.0	340	29.43	733	5.0	261.8	321.7	320.6
14.98	427	29.44	744	10.0	334.4	424.0	417.0
20.0	532	40.35	980	13.4	380.9	471.3	460.6
24.97	631	40.35	992	18.0	440.5	536.1	-
30.0	744	40.35	1005	19.4	458.5	-	539.0
40.05	1005	49.59	1253	21.2	494.3	-	566.1
50.04	1301			25.0	596.0	708.6	666.1
60.03	1653			30.5	666.6	810.6	761.8
70.0	1987						
80.0	2400						
25.0	622						
eq 6	P/(mmHg·L/mol)						
A	73.022						
B	22.261						
C	4254.8						

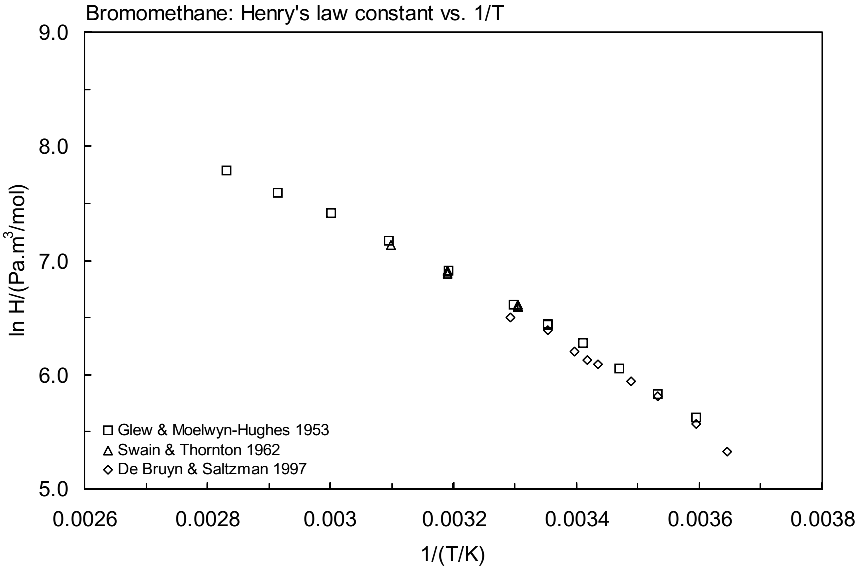
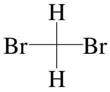


FIGURE 5.1.2.1.2 Logarithm of Henry's law constant versus reciprocal temperature for bromomethane.

5.1.2.2 Dibromomethane



Common Name: Dibromomethane
Synonym: methylene bromide
Chemical Name: dibromomethane, methylene bromide
CAS Registry No: 74-95-3
Molecular Formula: CH_2Br_2
Molecular Weight: 173.835
Melting Point (°C):
  –52.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
  97.0 (Horvath 1982; Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
  2.4970, 2.4842 (20°C, 25°C, Dreisbach 1961)
  2.4970 (Horvath 1982; Weast 1982–83)
Molar Volume (cm^3/mol):
  70.1 (Stephenson & Malanowski 1987)
  76.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  11480* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
  11700, 11930 (15°C, 30°C, shake flask-interferometer, Gross & Saylor 1931)
  11486 (Seidell 1940; quoted, Deno & Berkheimer 1960)
  17500 (shake flask-residue volume method, Booth & Everson 1948)
  11000 (O'Connell 1963; Jolles 1966)
  11442* (summary of literature data, Horvath 1982)
  11500 (Dean 1985)
  12800*, 11400 (19.3°C, 29.5°C, shake flask-GC/TC, measured range 0–90.1°C, Stephenson 1992)
  11420, 12030, 12270, 12580 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
  11114, 12060, 13052 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
  12300 (20°C, limiting activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  4626, 7518 (20°C, 30°C, Rex 1906)
  5775* (Antoine eq. regression, temp range –35.1 to 98.6°C, Stull 1947)
  6034 (calculated by formula, Dreisbach 1961)
  $\log (P/mmHg) = 7.0625 - 1327.8/(220.58 + t/°C)$; temp range 17–236°C (Antoine eq. for liquid state, Dreisbach 1961)
  5767 (calculated-Antoine eq., Weast 1972–73)
  $\log (P/mmHg) = [-0.2185 \times 8722.0/(T/K)] + 8.028019$; temp range –35.1 to 98.6°C (Antoine eq., Weast 1972–73)
  5922 (Antoine eq. regression, Kudchadker et al. 1979)
  $\log (P/mmHg) = 7.82594 - 1784.9/(263.73 + t/°C)$ (Antoine eq., Kudchadker et al. 1979)
  6034 (calculated-Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_L/kPa) = 6.1874 - 1327.8/(-52.57 + T/K)$; temp range 290–409 K (Antoine eq., Stephenson & Malanowski 1987)

4650, 7730, 9840, 12383 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 35.3525 – 3.0445 × 10^3/(T/K) –9.5792·log (T/K) + 5.8258 × 10^{-10}·(T/K) + 2.9443 × 10^{-6}·$(T/K)^2$; temp range 221–611 K (vapor pressure eq., Yaws 1994)
6084.6 (selected and summary of literature data, temp range 220.61–413.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
90.0 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
73.16 (calculated-bond method, Hine & Mookerjee 1975)
86.13 (batch stripping-GC, Nicholson et al. 1984)
86.03 (Munz & Roberts 1989)
70.9, 111.5, 142, 172 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
72.7, 141, 252 (20, 30, 40°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
281, 513 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
25.4, 48.3, 81.9 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
ln K_{AW} = 11.70 – 4418/(T/K); seawater of salinity of 30.4‰, temp range 0–20°C (Moore et al. 1995)
66.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
68.94 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated:
2.50 (Hansch et al. 1968)
1.70 (recommended, Sangster 1993)
1.70 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)
1.70, 1.65, 1.64 (25, 35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
1.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
3.07 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 4.1 ppm/min-g of catalyst (Ollis 1985).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k(aq.) = (6.1 ± 0.61) × 10^{-7} M^{-1} s^{-1} was measured in 66.7% dioxane-water at 35.7°C (Hine et al. 1956; quoted, Roberts et al. 1992)
k_{OH} = 2.5 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} and estimated residence time of 46 d at 300 K (Singh et al. 1980)
k_{OH} = 5 × 10^{11} cm^3 mol^{-1} s^{-1}, estimated at 300 K (Lyman 1982)
k(aq.) = 4.0 × 10^{-7} M^{-1} s^{-1} for the reaction with OH radical in aqueous solution with reference to CH_3CCl_3 (Buxton et al. 1988; quoted, Haag & Yao 1992)
k_{O3}(aq.) ≤ 0.005 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21°C, with $t_{½}$ ≥ 80 d at pH 7 (Yao & Haag 1991).
k_{OH}(aq.) = (9.0 ± 3.0) × 10^{-7} M^{-1} s^{-1} for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)
Hydrolysis: rate constant k = 1.2 × 10^{-10} s^{-1} with $t_{½}$ = 183 yr at pH 7 and 25°C (Mabey & Mill 1978)
$t_{½}$ = 183 yr at pH 7 and 25°C, based on overall hydrolysis rate constant (Mill et al. 1982; quoted, Howard et al. 1991).
Biodegradation:
k = 2.1 × 10^{-4} min^{-1} with $t_{½}$ = 24 min in anoxic sediment-water suspension (Jafvert & Wolfe 1987)

$t_{1/2}$(aq. aerobic) = 168–672 h, based on unacclimated aerobic screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2}$(aq. anaerobic) = 672–2688 h, based on unacclimated aqueous aerobic half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

estimated as toxic chemical residence time of 46 d with rate constant of 2.5×10^{-13} cm^3 molecule^{-1} s^{-1} for the reaction with OH radical at 300 K (Singh et al. 1980);

photooxidation $t_{1/2}$ = 851–8510 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 183 yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{1/2}$ = 55 h in anoxic sediment-water suspension (Jafvert & Wolfe 1987);

$t_{1/2}$ = 168-672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured $k \leq 0.005$ M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21°C, with $t_{1/2} \geq 80$ d at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2}$ = 336-1344 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2}$ = 55 h in anoxic Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

Soil: $t_{1/2}$ = 168–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.2.2.1
Reported aqueous solubilities of dibromomethane at various temperatures

$$S/(wt\%) = 1.1594 - 4.3267 \times 10^{-3} \cdot (t/°C) + 1.8201 \times 10^{-4} \cdot (t/°C)^2 - 1.3335 \times 10^{-6} \cdot (t/°C)^3 \quad (1)$$

1.

Rex 1906		Horvath 1982		Stephenson 1992		Tse et al. 1992	
volumetric method		summary of literature data		shake flask-GC		activity coefficient	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	11730	5	11594	0	11700	20	11420
10	11460	10	11330	9.7	11300	30	12030
20	11480	20	11350	19.3	12800	35	12270
30	11760	25	11442	29.5	11400	40	12580
		30	11574	39.5	12000		
				49.5	12700		
				59.9	13600		
				69.9	13600		
				79.8	16100		
				90.1	15100		

Gross & Saylor 1931	
shake flask-interferometer	
t/°C	S/g·m^{-3}
15	11700
30	11930

Wright et al. 1992	
activity coefficient	
t/°C	S/g·m^{-3}
20	11114
30	12060
40	13052

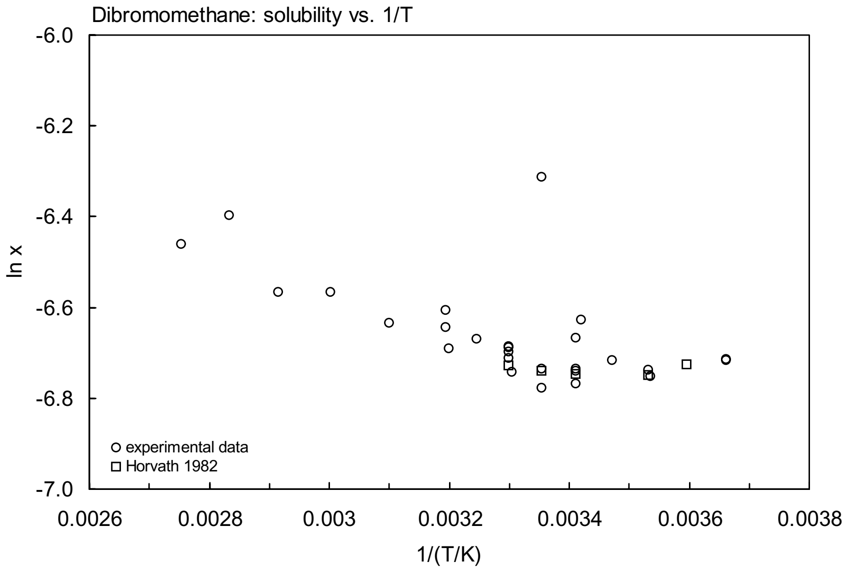


FIGURE 5.1.2.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for dibromomethane.

TABLE 5.1.2.2.2
Reported vapor pressures of dibromomethane at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
–35.1	133.3
–13.2	666.6
–2.40	1333
9.70	2666
23.3	5333
31.6	7999
42.3	13332
58.5	26664
79.0	53329
98.6	101325
mp/°C	–52.8

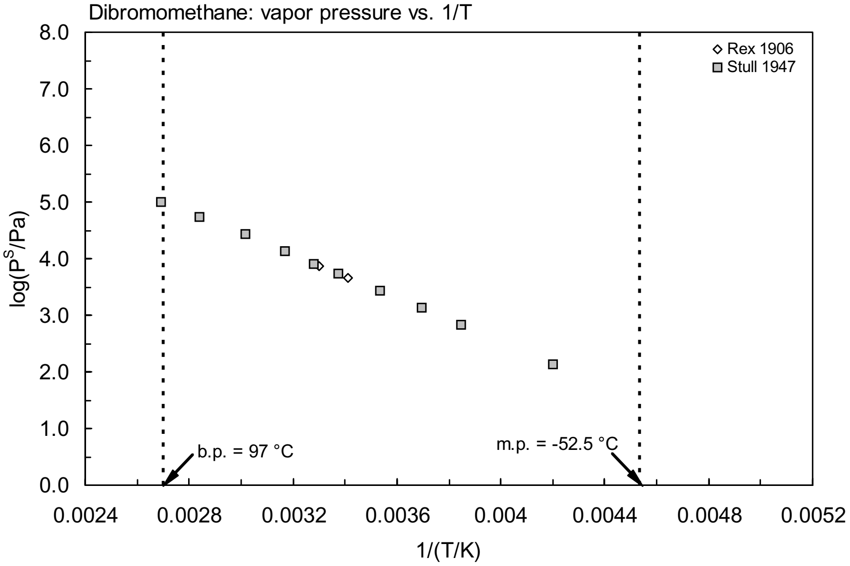


FIGURE 5.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for dibromomethane.

TABLE 5.1.2.2.3
Reported Henry's law constants of dibromomethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/atm) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Tse et al. 1992		Wright et al. 1992		Bhatia & Sandler 1995		Moore et al. 1995	
activity coefficient		activity coefficient		activity coefficient		gas stripping-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
						seawater, salinity 30.4‰	
20	70.9	20	72.7	35	281	0	25.4
30	111.5	30	141	50	513	10	48.3
35	142	40	252			20	81.9
40	172						
						eq. 1	K_{AW}
						A	11.70 ± 0.03
						B	4418 ± 154

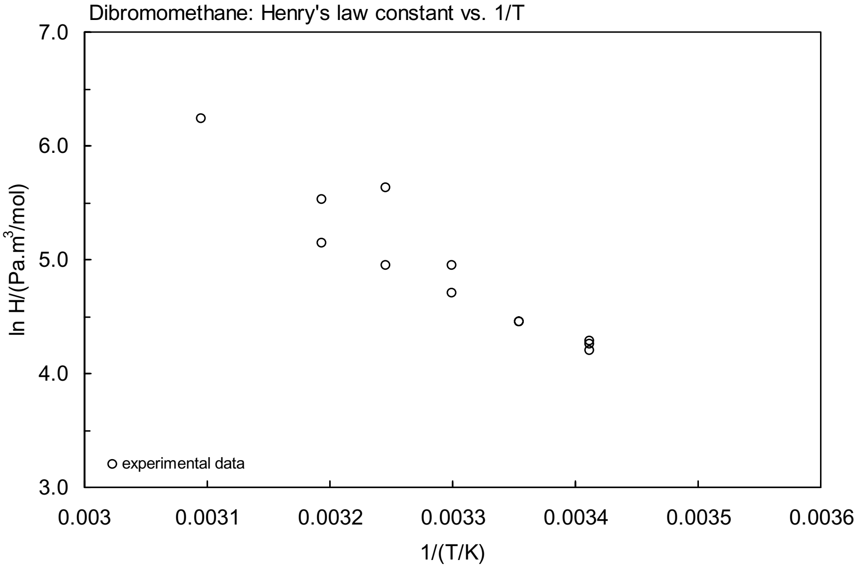
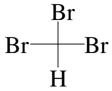


FIGURE 5.1.2.2.3 Logarithm of Henry's law constant versus reciprocal temperature for dibromomethane.

5.1.2.3 Tribromomethane



$\mathrm{Br}-\overset{\mathrm{Br}}{\underset{\mathrm{H}}{|}}-\mathrm{Br}$

Common Name: Tribromomethane
Synonym: bromoform, methenyl tribromide
Chemical Name: tribromomethane
CAS Registry No: 75-25-2
Molecular Formula: $CHBr_3$
Molecular Weight: 252.731
Melting Point (°C):
8.69 (Lide 2003)
Boiling Point (°C):
149.1 (Lide 2003)
Density (g/cm^3 at 20°C):
2.8910 (Kahlbaum & Arndt 1898; Riddick et al. 1986)
2.8917, 2.8909 (Kudchadker et al. 1979)
Molar Volume (cm^3/mol):
87.42 (20°C, calculated-density)
99.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
3010, 3190 (15°C, 30°C, shake flask-interferometer, Gross & Saylor 1931)
3110 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
3190 (30°C, Seidell 1941)
3033 (Verschueren 1977)
3100 (recommended, Horvath 1982)
3931 (30°C, headspace-GC, McNally & Grob 1984)
3200 (30°C, Dean 1985)
3180 (30°C, selected, Riddick et al. 1986)
3235, 3452, 3695 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
3978, 4555, 3467 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
3163 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
987* (30°C, temp range 30–110°C, Kireev & Simnikow 1941; quoted, Boublik et al. 1984)
667* (22°C, summary of literature data, temp range 22–150.5°C, Stull 1947)
2453* (47.207°C, temp range 47.207–139.055°C, Boublik & Aim 1972; quoted, Boublik et al. 1984)
815 (calculated-Antoine eq., Weast 1972–73)
$\log (P/\mathrm{mmHg}) = [-0.2185 \times 9673.3/(T/K)] + 7.875367$; temp range 22–150°C (Antoine eq., Weast 1972–73)
715 (calculated-Antoine eq., Boublik et al. 1973)
$\log (P/\mathrm{mmHg}) = 6.82182 - 1376.748/(200.966 + t/°C)$; temp range 30–100°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
720 (calculated-Antoine eq., Kudchadker et al. 1979)
$\log (P/\mathrm{mmHg}) = 7.03141 - 1511.50/(214.21 + t/°C)$ (Antoine eq., Kudchadker et al. 1979)
717 (calculated-Antoine eq., Boublik et al. 1984)
$\log (P/\mathrm{kPa}) = 5.97839 - 1294.382/(202.729 + t/°C)$; temp range 30–100.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 6.8218 – 1376.7/(201.0 + t/°C); temp range 30–101°C (Antoine eq., Dean 1985, 1992)
790 (quoted, Riddick et al. 1986)
727 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.20911 – 1544.81/(–54.77 + T/K); temp range 320–412 K (Antoine eq., Stephenson & Malanowski 1987)
543, 981, 1704(20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = –10.2943 – 2.170 × 10^3/(T/K) + 9.1193·log (T/K) – 1.6495 × 10^{-2}·(T/K) + 7.4917 × 10^{-6}·$(T/K)^2$; temp range 281–696 K (vapor pressure eq., Yaws 1994)
685.5 (selected and summary of literature data, temp range 281.2–478.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
68.3 (calculated-1/K_{AW}, C_W/C_A, Hine & Mookerjee 1975)
7.66 (calculated-bond method, Hine & Mookerjee 1975)
62.3, 62.0 (calculated-P/C, recommended, Mackay & Shiu 1981,1990)
56.7 (20°C, calculated-P/C, Mabey et al. 1982)
43.6, 43.6; 58.8 (20°C, batch stripping-GC, calculated-P/C, distilled water, Nicholson et al. 1984)
46.6, 41.54, 43.6 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)
ln [H/(atm m^3/mol)] = 116.0 – 5670/(T/K); temp range 10–30°C (air stripping-GC, Nicholson et al. 1984)
54.2 (EPICS-LSC, Munz & Roberts 1987, 1989)
log K_{AW} = 4.729 – 1905/(T/K); temp range 10–30°C (EPICS-LSC measurements, Munz & Roberts 1987)
53.9 (gas stripping-GC, Warner et al. 1987)
56.7 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
40.5, 70.9, 122 (20, 30, 40°C, infinite dilution activity coeff. γ^∞-GC, Tse et al. 1992)
34.0, 71.6, 207 (20, 35, 50°C, activity coeff. γ^∞-differential pressure transducer, Wright et al. 1992)
43.6 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
182, 536 (10, 20°C, gas stripping-GC, Moore et al. 1995)
14.3, 29.2, 52.9 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
ln K_{AW} = 13.16 – 4973/(T/K); seawater of salinity of 30.4‰, temp range: 0–20°C (Moore et al. 1995)
42.65 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 5.476 – 2120/(T/K) (summary of literature data, Staudinger & Roberts 2001)
104.4 (37°C, equilibrium headspace-GC, Batterman et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
2.30 (calculated as per Tute 1971, Callahan et al. 1979)
2.38 (calculated-f const., Mabey et al. 1982; Valsaraj 1988)
2.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
1.80 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
2.07 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization: calculated $t_{½}$ = 63 min to 24.2 d (using Langbein & Durum 1967 published O_2 reaeration values) and $t_{½}$ = 65.6 d both from rivers and streams (Kaczmar et al. 1984).
Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 6.2 ppm/min per gram of catalyst (Ollis 1985).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k << 360 M^{-1} h^{-1} for singlet oxygen and k = 0.5 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation $t_{½}$ = 1299–12989 h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

k = 4.0 × 10^7 M^{-1} s^{-1} for reaction with OH radical in water with reference to CH_3CCl_3 (Buxton et al. 1988; quoted, Haag & Yao 1992)

k_{OH}(aq.) = (1.3 ± 0.6) × 10^8 M^{-1} s^{-1} for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

Hydrolysis: a maximum $t_{½}$ = 686 yr has been estimated at pH 7 and 25°C from experimental data at 100–150°C (Radding et al. 1977) which corresponds to a first-order rate constant k = 3.2 × 10^{-11} s^{-1} (Radding et al. 1977; Mabey & Mill 1978; quoted, Mabey et al. 1982; Howard et al. 1991);

rate constant k = 3.2 × 10^{-11} s^{-1} with $t_{½}$ = 686 yr at pH 7 and 25°C (Mabey & Mill 1978)

rate constant k = 2.5 × 10^{-9} h^{-1} assigned by analogy to trichloromethane (Mabey et al. 1982).

Biodegradation: $t_{½}$ = 672–4320 h in soil, based on unacclimated aerobic aqueous screening test data from experiments utilizing settled domestic wastewater inoculum (Bouwer et al. 1984; quoted, Howard et al. 1991); anaerobic $t_{½}$ = 2688–17280 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated rate constant k ~ 1 × 10^{-10} mL $cell^{-1}$ h^{-1} for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{½}$ = 1299–12989 h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 686 yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

Ground water: $t_{½}$ = 1344–8640 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 672–4320 h, based on unacclimated aerobic aqueous screening test data from experiments utilizing settled domestic wastewater inoculum (Bouwer et al. 1984; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.2.3.1
Reported aqueous solubilities of tribromomethane at various temperatures

Gross & Saylor 1931		Tse et al. 192		Wright et al. 1992	
shake flask-interferometer		activity coefficient		activity coefficient	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
15	3010	20	3235	20	3978
30	3190	30	3452	35	4555
		40	3695	50	3467

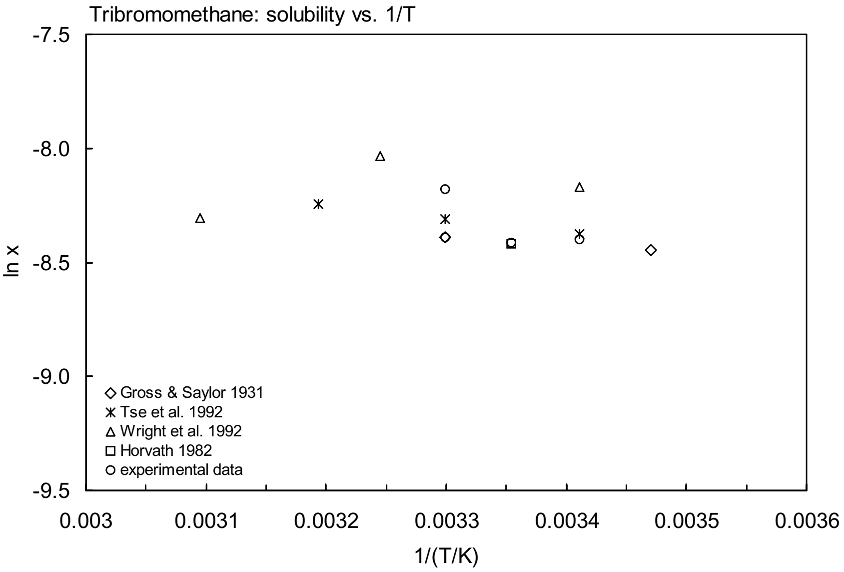


FIGURE 5.1.2.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for tribromomethane.

TABLE 5.1.2.3.2
Reported vapor pressures of tribromomethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log(T/K)$ (4)

Kireev & Simnikow 1941		**Stull 1947**		**Boublik & Aim 1972**			
in Boublik et al. 1984		**summary of literature data**		**in Boublik et al. 1984**			
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
30.0	987	-	133.3	47.207	2453	123.929	49704
35.0	1267	22.0	666.6	59.767	4524	130.982	61295
40.0	1747	34.0	1333	69.518	6967	139.055	77125
50.0	2946	48.0	2666	76.389	9306	bp/°C	78.177
60.0	4693	63.6	5333	82.821	12046		at 10 mmHg
70.0	7399	73.4	7999	87.709	14549	Antoine eq.	
80.0	11306	85.9	13332	93.356	17921	eq. 2	P/kPa
90.0	16852	106.1	26664	98.173	21314	A	6.20467
110.0	24198	127.9	53329	103.595	25780	B	1541.946
		150.5	101325	108.003	29923	C	218.084
				113.216	35493		
		mp/°C	8.5	118.078	41470		

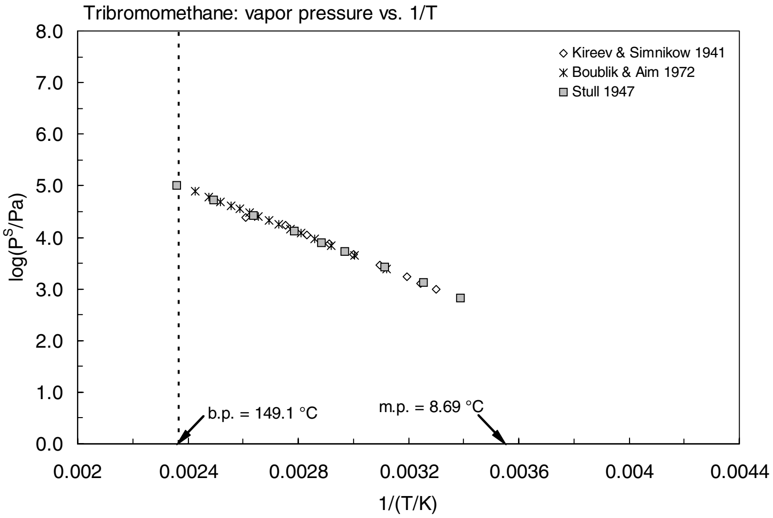


FIGURE 5.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for tribromomethane.

5.1.2.4 Bromoethane (Ethyl bromide)

Common Name: Ethyl bromide
Synonym: bromoethane, monobromoethane
Chemical Name: ethyl bromide, bromoethane
CAS Registry No: 74-96-4
Molecular Formula: C_2H_5Br, CH_3CH_2Br
Molecular Weight: 108.965
Melting Point (°C):
–118.60 (Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
38.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.4594, 1.4492 (20°C, 25°C, Dreisbach 1959)
1.4505 (25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
75.12 (calculated from density)
75.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
27.55, 26.48 (25°C, at bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
5.858 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
9140* (20°C volumetric method, measured range 0–30°C, Rex 1906)
9600 (17.5°C, volumetric method, Führer 1924)
8880 (30°C, van Arkel & Vles 1936)
9064 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
9000 (shake flask-interferometry, Donahue & Bartell 1952)
8939* (summary of literature data, temp range 0–30°C, Horvath 1982)
9100 (Dean 1985; Riddick et al. 1986)
9000* (tentative value, temp range 0–°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
$S/(wt\%) = 13.2481 - 8.0012 \times 10^{-2}\cdot(T/K) + 1.29448 \times 10^{-4}\cdot(T/K)^2$, temp range 273–303 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
51440, 75140 (20°C, 30°C, Rex 1906)
70095* (28.145°C, temp range 28.145–75.365°C, Zmaczynski 1930)
53329* (21°C, summary of literature data, temp range –74.3 to 38.4°C, Stull 1947)
62460 (calculated-Antoine eq., Dreisbach 1959)
$\log (P/mmHg) = 6.91995 - 1090.81/(231.71 + t/°C)$; temp range –32 to 110°C (Antoine eq. for liquid state, Dreisbach 1959)
$\log (P/mmHg) = 6.91995 - 1090.810/(231.71 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
$\log (P/mmHg) = [-0.2185 \times 6843.1/(T/K)] + 7.635277$; temp range 74.3 to 229.5°C (Antoine eq., Weast 1972–73)
62230 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 6.11352 - 1121.957/(234.741 + t/°C)$; temp range 28.145–75.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 6.9886 – 1121.9/(234.7 + t/°C); temp range 28–75°C (Antoine eq., Dean 1985, 1992)
62470 (lit; average, Riddick et al. 1986)
log (P/kPa) = 6.04485 – 1090.81/(231.71 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
62470 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.04485 – 1090.81/(–41.44 + T/K); temp range 225–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.66835 – 1151.96/(12.999 + T/K); temp range 334–504 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.77490 – 1602.405/(25.282 + T/K); temp range 326–454 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.99873 – 1619.697/(T/K); temp range 452–503 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 38.1816 – 2.517×10^3/(T/K) – 10.329·log (T/K) – 2.3368×10^{-10}·(T/K) + 5.4956×10^{-6}·$(T/K)^2$; temp range 155–504 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

766	(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
751	(computed value, Yaws et al. 1991)
767	(γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

1.60	(calculated-π const., Hansch et al. 1968)
1.61	(shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979, 1987)
1.61	(recommended, Sangster 1989)
1.61	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{AW} at 25°C:

1.53	(calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: k = 2.64×10^{-7} s^{-1} with $t_{1/2}$ ~ 30 d at pH 7 and 25°C (Mabey & Mill 1978)
k = 9.4×10^{-4} h^{-1} at pH 7 and 25°C with $t_{1/2}$ ~ 30 d (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).
Surface water: $t_{1/2}$ ~ 30 d at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

TABLE 5.1.2.4.1
Reported aqueous solubilities of bromoethane at various temperatures

$$S/(\text{wt\%}) = 1.0557 - 0.01309\cdot(t/°C) + 3.3850 \times 10^{-4}\cdot(t/°C)^2 - 2.950 \times 10^{-6}\cdot(t/°C)^3 \quad (1)$$

$$S/(\text{wt\%}) = 13.2481 - 8.0012 \times 10^{-2}(T/K) + 1.29448 \times 10^{-4}\cdot(T/K)^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
0	10670	0	10557	0	10510
10	9650	10	9557	5	10080
20	9140	20	9057	10	9710
30	8960	25	8939	15	9410
		30	8880	20	9170
				25	9000
		eq. 1	S/wt%	30	8890
				eq. 2	S/wt%
				temp range 273–303 K	

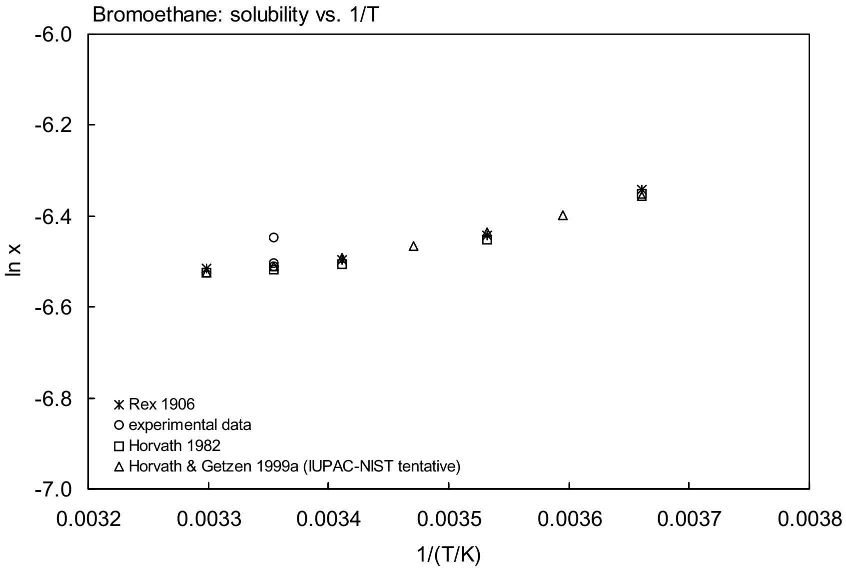


FIGURE 5.1.2.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for bromoethane.

TABLE 5.1.2.4.2
Reported vapor pressures of bromoethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Zmaczynski 1930		Stull 1947	
		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
28.145	70095	–74.3	133.3
33.247	83515	–56.4	666.6
43.560	120803	–47.5	1333
48.771	143268	–37.8	2666
54.018	169066	–26.7	5333
59.300	198543	–19.5	7999
64.619	232113	–10.0	13332
69.94	270150	4.50	26664
75.365	312960	21.0	53329
		38.4	101325
		mp/°C	–117.8

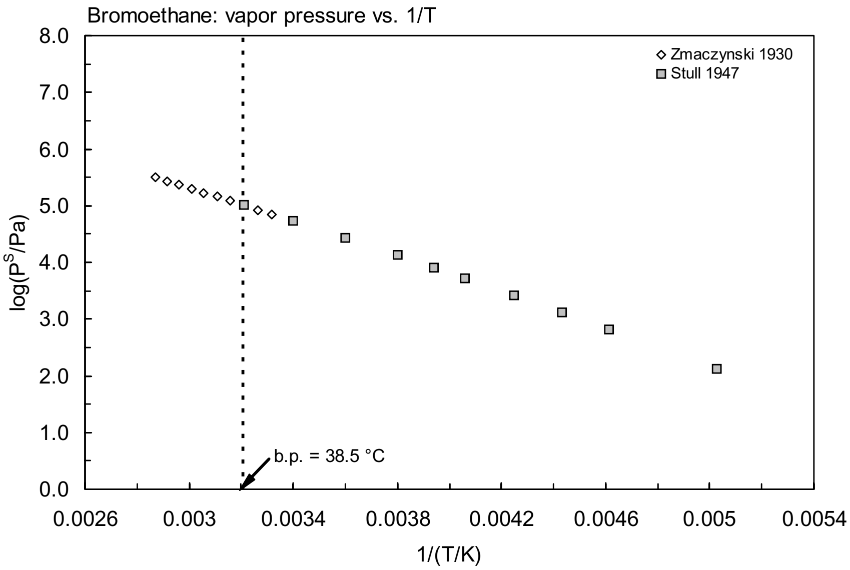
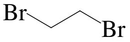


FIGURE 5.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for bromoethane.

5.1.2.5 1,2-Dibromoethane



Common Name: 1,2-Dibromoethane
Synonym: ethylene bromide, ethylene dibromide, *sym*-dibromoethane, EDB
Chemical Name: 1,2-dibromoethane
CAS Registry No: 106-93-4
Molecular Formula: $C_2H_4Br_2$, CH_2BrCH_2Br
Molecular Weight: 187.861
Melting Point (°C):
9.84 (Lide 2003)
Boiling Point (°C):
131.6 (Lide 2003)
Density (g/cm^3 at 20°C):
2.1792, 2.1688 (20°C, 25°C, Dreisbach 1959; Horvath 1982)
2.1791, 2.1687 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
86.25 (20°C, calculated-density, Stephenson & Malanowski 1987)
98.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
41.73, 36.35 (25°C, at bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
10.03 (calculated, Dreisbach 1959)
10.945 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
3920, 4310 (15°C, 30°C, shake flask-interferometer, Gross & Saylor 1931)
4040* (measured range 0–50°C, van Arkel & Vles 1936)
4017 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
8600 (shake flask-volumetric method, Booth & Everson 1948)
4200 (measured by Dow Chemical, Dreisbach 1959)
3510* (20°C, shake flask-GC, measured range 3–34°C, Chiou & Freed 1977)
2910 (shake flask-GC, Jones et al. 1977/78)
3520 (shake flask-GC, Chiou et al. 1979)
4320, 4321 (20°C, 25°C, shake flask-GC, Mackay et al. 1980)
4152* (summary of literature data, Horvath 1982)
4310 (30°C, Verschueren 1983)
4290 (30°C, selected, Riddick et al. 1986)
3120 (shake flask-reverse phase polarography, Tokoro et al. 1988)
4120*, 4310 (19.5°C, 30.7°C, shake flask-GC/TC, measured range 10.0–90.6°C, Stephenson 1992)
4192 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
3910* (tentative value, temp range 0–75°C. IUPAC-NIST Solubility Data Series, Hovath & Getzen 1999a)
$S/(wt\%) = 3.8651 - 2.7921 \times 10^{-2} \cdot (T/K) + 5.45647 \times 10^{-5} \cdot (T/K)^2$, temp range 273–348 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1333 (18.2°C, summary of literature data, temp range –27 to 131.1°C, Stull 1947)
1560 (calculated-Antoine eq., Dreisbach 1959)
$\log (P/mmHg) = 7.06245 - 1469.7/(220.0 + t/°C)$; temp range 43–215°C (Antoine eq. for liquid state, Dreisbach 1959)

log (P/mmHg) = [–0.2185 × 9229.4/(T/K)] + 7.93581; temp range –27 to 304°C (Antoine eq., Weast 1972–73)
1466, 2266 (20°C, 30°C, Verschueren 1983)
1626 (interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.62666 – 1156.346/(2187.446 + t/°C); temp range 52.56–131.41°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.72148 – 1280.82/(201.75 + t/°C); temp range 52–131°C (Antoine eq., Dean 1985, 1992)
1540 (lit. average, Riddick et al. 1986)
log (P/kPa) = 4.32297 – 1560.3/(230.0 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
log (P_S/kPa) = 10.03 – 2863/(T/K); temp range 228–248 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 9.009 – 2606.5/(T/K); temp range 251–281 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.501– 2181.1/(T/K); temp range 283–317 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.18375 – 1469.7/(–53.15 + T/K); temp range 316–488 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.16941 – 3200/(117.25 + T/K); temp range 404–578 K (Antoine eq.-V, Stephenson & Malanowski 1987)
log (P/mmHg) = 16.8759 – 2.4267 × 10^3/(T/K) –3.0891·log (T/K) – 6.0088 × 10^{-10}·(T/K) + 3.5901 × 10^{-7}·$(T/K)^2$; temp range 283–650 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
71.49 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
15.64, 110.7 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)
65.86* (EPICS-GC, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm m^3 mol^{-1})] = 5.703 – 3876/(T/K); temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)
71.49, 133.12 (quoted, calculated-QSAR, Nirmalakhandan & Speece 1988)
83.07 (20–25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)
70.77 (computed value, Yaws et al. 1991)
52.6 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
52.02 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
54.84 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 3.661 – 1556/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
1.96 (shake flask, Log P Database, Hansch & Leo 1987)
1.96 (recommended, Sangster 19943)
1.96 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
0.778 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
0.301 (calculated-K_{OC} as per Kenaga & Goring 1978, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
1.556 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
1.643 (soil, quoted, Kenaga 1980; Kenaga & Goring 1980)
1.699 (soil, calculated as per Kenaga & Goring 1978, Kenaga 1980)
1.643 (soil, selected, Jury et al. 1990)
1.64 (soil, organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k and Half-Lives, $t_{½}$:
Volatilization: estimated volatilization $t_{½}$ ~ 6.1 h from water (Thomas 1982)
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH} = 2.5 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow system, Howard & Evenson 1976)

k_{OH}(calc) = 2.9 × 10^{-13} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 2.5 × 10^{-13} cm^3 molecule^{-1} s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1985)

k_{OH} = 2.5 × 10^{-13} cm^3 molecule^{-1} s^{-1} with a loss rate of 0.01 d^{-1}, k_{O3} < 10^{-23} cm^3 molecule^{-1} s^{-1} with a loss rate of < 6 × 10^{-7} d^{-1} at room temp. (Atkinson 1985)

k_{O3}(aq.) ≤ 0.014 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with a half-life of 28 d at pH 7 (Yao & Haag 1991).

Hydrolysis: EDB hydrolyzes to ethylene glycol and bromoethanol in water at pH 7 and 25°C with $t_{½}$ = 5–10 d (Leinster et al. 1978; quoted, Verschueren 1983);

k = 9.9 × 10^{-6} h^{-1} at pH 7 and 25°C with a calculated $t_{½}$ = 8.0 yr (Jungclaus & Cohen 1986; quoted, Ellington 1989);

rate constant k = (8.9 ± 0.1) × 10^{-9} s^{-1} in water at 25°C and pH 7.5 with an estimated half-life of 2.5 yr (Vogel & Reinhard 1986);

$t_{½}$ = 2.2 yr, based on measured neutral hydrolysis rate constant at pH 7 and 25°C (Weintraub et al. 1986; quoted, Howard et al. 1991).

Biodegradation: aerobic $t_{½}$(aq.) = 672–4320 h, based on unacclimated aqueous aerobic biodegradation screening test data (Bouwer & McCarty 1983; quoted, Howard et al. 1991);

anaerobic $t_{½}$(aq.) = 48–360 h, based on anaerobic stream and pond water sediment die-away test data (Jafvert & Wolfe 1987; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976); photooxidation $t_{½}$ = 257–2567 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 672–4320 h, based on unacclimated aqueous aerobic biodegradation (Howard et al. 1991);

k(exptl) ≤ 0.014 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{½}$ ≥ 28 d at pH 7 (Yao & Haag 1991).

Ground water: $t_{½}$ = 470–2880 h, based on data from anaerobic ground water ecosystem study (Wilson et al. 1986; quoted, Howard et al. 1991) and data from an aerobic ground water ecosystem study (Swindoll et al. 1987; quoted, Howard et al. 1991).

Sediment: calculated $t_{½}$ = 1500 d at 25°C and pH 7, based on studies in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil: estimated $t_{½}$ ~ 3650 d of volatilization loss from soil (Jury et al. 1990);

disappearance $t_{½}$ < 2.0 d, estimated from the volatilization loss of mixtures (Anderson et al. 1991);

$t_{½}$ = 672–4320 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.2.5.1
Reported aqueous solubilities of 1,2-dibromoethane at various temperatures

$$S/(wt\%) = 0.36583 + 1.4836 \times 10^{-3}\cdot(t/°C) + 3.48175 \times 10^{-6}\cdot(t/°C)^2 + 6.47685 \times 10^{-7}\cdot(t/°C)^3 \quad (1)$$

$$S/(wt\%) = 3.8651 - 2.7921 \times 10^{-2}\cdot(T/K) + 5.45647 \times 10^{-5}\cdot(T/K)^2, \quad (2)$$

1.

Gross & Saylor 1931		van Arkel & Vles 1936		Chiou & Freed 1977		Horvath 1982	
shake flask-interferometer				shake flask-GC		summary of literature data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
15	3920	0	3340	3	2960	5	3658
30	4310	20	4020	20	3510	10	3817
		35	4490	34	4150	20	4012
		50	5290			25	4152

(Continued)

TABLE 5.1.2.5.1 (*Continued*)

Gross & Saylor 1931		van Arkel & Vles 1936		Chiou & Freed 1977		Horvath 1982	
shake flask-interferometer				shake flask-GC		summary of literature data	
t/°C	$S/g{\cdot}m^{-3}$	t/°C	$S/g{\cdot}m^{-3}$	t/°C	$S/g{\cdot}m^{-3}$	t/°C	$S/g{\cdot}m^{-3}$
						30	4310
						40	4722
						50	5297
						60	6073
						70	7089
						80	8384
						eq.1	S/wt%

2.

Stephenson 1992		Horvath & Getzen 1999a			
shake flask-GC		tentative, IUPAC-NIST			
t/°C	$S/g{\cdot}m^{-3}$	t/°C	$S/g{\cdot}m^{-3}$	t/°C	$S/g{\cdot}m^{-3}$
				continued	
10.1	3950	0	3090	55	5780
19.5	4120	5	3200	60	6190
30.7	4310	10	3340	65	6630
39.6	4440	15	3500	70	7090
50	4930	20	3690	75	7580
59.9	4890	25	3910		
70.2	5420	30	4150	eq. 2	S/wt%
80.3	5720	35	4420		
90.6	6580	40	4720		
		45	5050		
		50	5400		

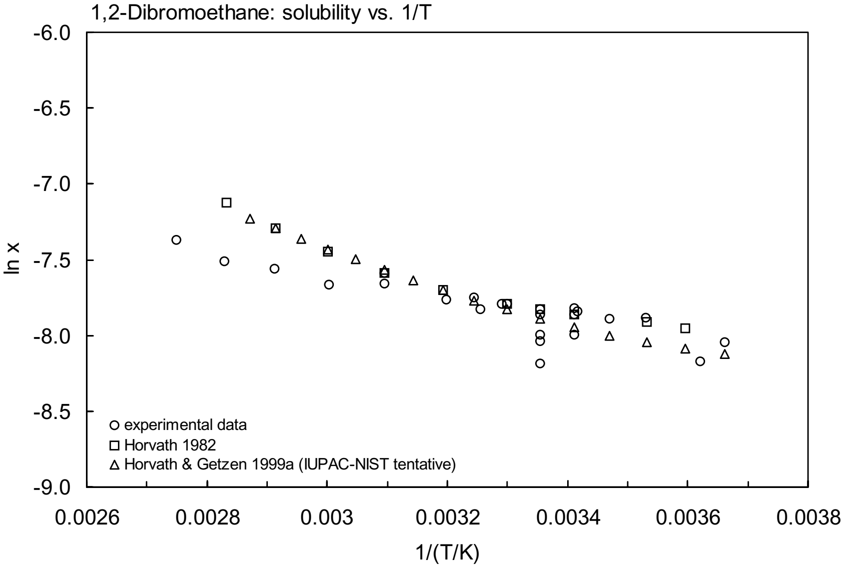


FIGURE 5.1.2.5.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,2-dibromomethane.

TABLE 5.1.2.5.2
Reported Henry's law constants of 1,2-dibromoethane at various temperatures

Ashworth et al. 1988	
EPICS-GC	
t/°C	H/(Pa m³/mol)
10	30.4
15	48.6
20	61.8
25	65.9
30	81.1
ln [H/(atm·m3/mol)] = A – B/(T/K)	
A	5.703
B	3876

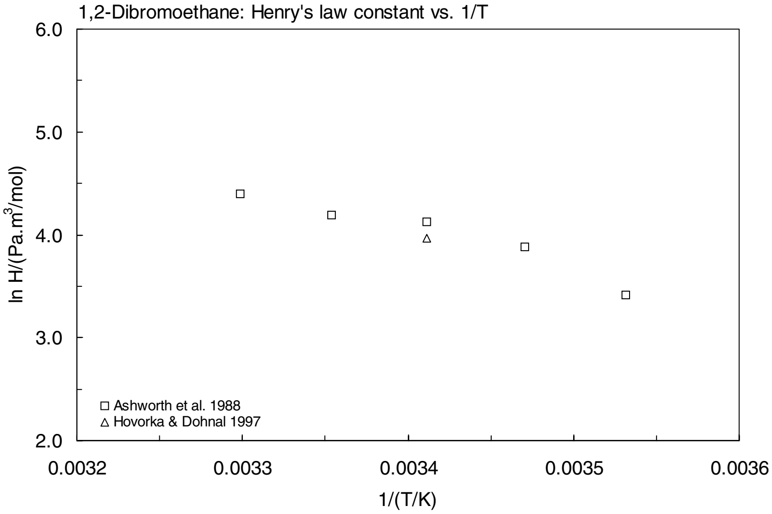
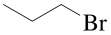


FIGURE 5.1.2.5.2 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dibromomethane.

5.1.2.6 1-Bromopropane



Common Name: 1-Bromopropane
Synonym: bromopropane, monobromopropane, *n*-propyl bromide, propyl bromide
Chemical Name: *n*-propyl bromide, 1-bromopropane
CAS Registry No: 106-94-5
Molecular Formula: C_3H_7Br, $CH_3CH_2CH_2Br$
Molecular Weight: 122.992
Melting Point (°C):
–110.3 (Lide 2003)
Boiling Point (°C):
71.1 (Lide 2003)
Density (g/cm^3 at 20°C):
1.3536, 1.3452 (20°C, 25°C, Dreisbach 1961)
1.3537 (Horvath 1982)
Molar Volume (cm^3/mol):
90.86 (20°C, calculated-density)
97.30 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
31.88, 68.8 (25°C, 68.8°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
9.037 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2450* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
2275 (19.5°C, shake flask, Fühner 1924)
2310 (30°C, shake flask-interferometer, Gross & Saylor 1931)
2312 (30°C, shake flask, Van Arkel & Vles 1936)
2454 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
2460 (calculated-K_{OW}, Hansch et al. 1968)
2450 (20°C, exptl., Korenman et al. 1971)
2427* (summary of literature data, Horvath 1982)
2300 (30°C, Dean 1985; Riddick et al. 1986)
2340* (tentative value, IUPAC-NIST Solubility Data Series, temp range 0–30°C Horvath & Getzen 1999)
$S/(wt\%) = 9.0608 - 0.05911\cdot(T/K) + 9.8925 \times 10^{-5}\cdot(T/K)^2$, temp range 273–303 K (Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
14770, 22740 (20°C, 30°C, volunmetric method Rex 1906)
13332* (18°C, summary of literature data, temp range –53.0 to 71°C, Stull 1947)
18440 (calculated by formula, Dreisbach 1961)
$\log (P/mmHg) = 6.91065 - 1194.889/(225.51 + t/°C)$; temp range –6 to 107°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = 6.91065 - 1194.889/(225.51 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
18300 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 6.09224 - 1232.529/(230.19 + t/°C)$; temp range 0–30°C (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)
18440 (selected, Riddick et al. 1986)
$\log (P/kPa) = 6.03960 - 1194.33/(225.223 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

log (P_L/kPa) = 6.03555 – 1194.889/(–47.64 + T/K); temp range 250–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.03823 – 1193.612/(–48.005 + T/K); temp range 301–344 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = $-9.0284 - 1.8916 \times 10^3/(T/K) + 9.691 \cdot \log (T/K) - 2.7013 \times 10^{-2} \cdot (T/K) + 1.7877 \times 10^{-5} \cdot (T/K)^2$; temp range 163–544 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

964.4	(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
1133, 1564	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
766.0	(calculated-QSAR, Nirmalakhandan & Speece 1988)
732	(computed value, Yaws et al. 1991)
950	(γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

2.10	(shake flask-GC, Fujita et al. 1964; Hansch & Anderson 1967; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)
2.10	(recommended, Sangster 1989, 1993)
2.10	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: k = 3.04×10^{-7} s^{-1} with estimated $t_{1/2}$ = 26 d at pH 7 and 25°C (Mabey & Mill 1978)
k = 1.1×10^{-3} h^{-1} at pH 7 and 25°C with estimated $t_{1/2}$ = 26 d.(Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).
Surface water: estimated $t_{1/2}$ = 26 d at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978
Ground water:
Sediment:
Soil:
Biota:

TABLE 5.1.2.6.1
Reported aqueous solubilities of 1-bromopropane at various temperatures

$$S/(\mathrm{wt}\%) = 0.2971 - 0.04225\cdot(t/°C) + 6.94998 \times 10^{-5}\cdot(t/°C)^2 + 5.00002 \times 10^{-7}\cdot(t/°C)^3 \quad (1)$$

$$S/(\mathrm{wt}\%) = 9.0608 - 0.05911\cdot(T/K) + 9.8925 \times 10^{-5}\cdot(T/K)^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
0	2980	0	2971	0	2980
10	2630	10	2623	5	2760
20	2450	20	2444	10	2580
30	2470	25	2427	15	2450
		30	2464	20	2370
				25	2340
		eq. 1	S/wt%	30	2360
				eq. 2	S/wt%
				temp range 273–303 K	

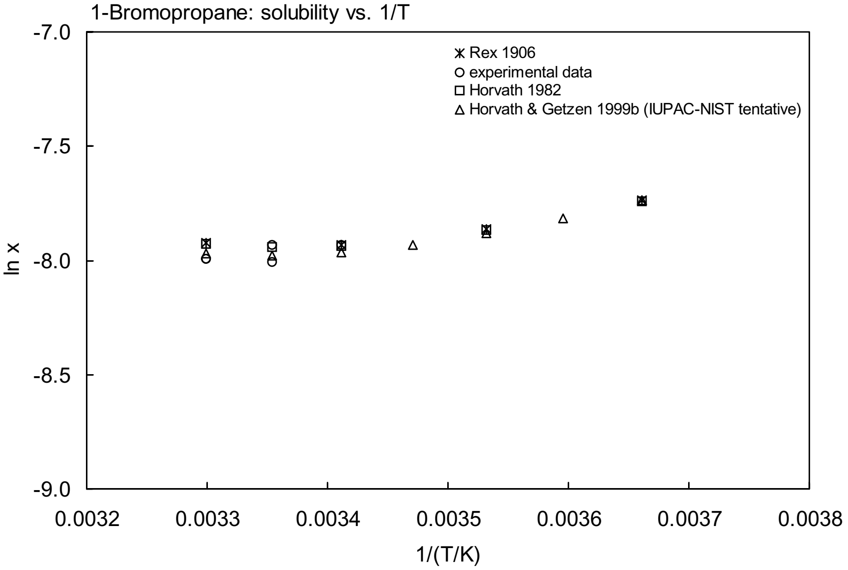


FIGURE 5.1.2.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1-bromopropane.

TABLE 5.1.2.6.2
Reported vapor pressures of 1-bromopropane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Rex 1906		Stull 1947	
		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
0	5546	–52.0	133.3
10	9091	–33.4	666.6
20	14772	–23.3	1333
30	22745	–12.4	2666
		–0.30	5333
		7.50	7999
		18.0	13332
		34.0	26664
		52.0	53329
		71.0	101325
		mp/°C	–109.0

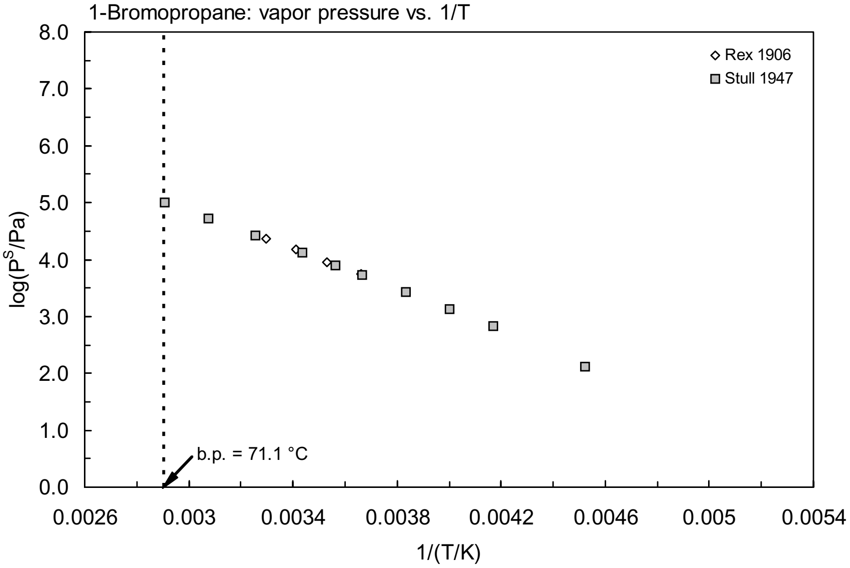
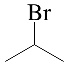


FIGURE 5.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1-bromopropane.

5.1.2.7 2-Bromopropane



Common Name: 2-Bromopropane
Synonym: isopropyl bromide
Chemical Name: 2-bromopropane, isopropyl bromide
CAS Registry No: 75-26-3
Molecular Formula: C_3H_7Br, $CH_3CHBrCH_3$
Molecular Weight: 122.992
Melting Point (°C):
  –89.0 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
  59.50 (Dean 1985; Lide 2003)
Density (g/cm^3 at 20°C):
  1.3140, 1.3060 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm^3/mol):
  93.6 (20°C, Stephenson & Malanowski 1987)
  97.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  30.16, 28.4 (25°C, 58.6°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  4180, 3650, 3180, 3180 (0, 10, 20, 30°C, volumetric method, Rex 1906)
  2877 (shake flask-volumetric method, Fühner 1924)
  3198 (30°C, shake flask, Van Arkel & Vles 1936)
  3162 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
  2880, 2690 (20°C, Korenman et al. 1971)
  3000 (selected exptl., Horvath 1982)
  2900 (18°C, Dean 1985)
  2860 (18°C, selected, Riddick et al. 1986)
  4160, 3640, 3170, 3170 (0, 10, 20, 30°C, tentative values of IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  23380, 35220 (20°C, 30°C, volumetric method Rex 1906)
  26664 (23.8°C, summary of literature data, temp range –61.8 to 60°C, Stull 1947)
  31500 (calculated by formula, Dreisbach 1961)
  $\log(P/mmHg) = 6.61405 - 1072.9/(228.0 + t/°C)$; temp range –19 to 95°C (Antoine eq. for liquid state, Dreisbach 1955)
  $\log(P/mmHg) = [-0.2185 \times 7591.7/(T/K)] + 7.887729$; temp range –61.8 to 60°C (Antoine eq., Weast 1972–73)
  28780 (interpolated-Antoine eq., Boublik et al. 1984)
  $\log(P/kPa) = 6.09819 - 1200.652/(233.815 + t/°C)$; temp range 0–30°C (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)
  31500 (selected, Riddick et al. 1986)
  $\log(P/kPa) = 5.92741 - 1106.82/(222.851 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
  31940 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
  $\log(P_L/kPa) = 5.28473 - 858.03/(-71.18 + T/K)$; temp range 236–328 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  $\log(P_L/kPa) = 5.91155 - 1098.573/(-51.268 + T/K)$; temp range 299–332 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 31.3032 - 2.4924 \times 10^3/(T/K) - 8.4645 \cdot \log(T/K) + 1.6459 \times 10^{-10} \cdot (T/K) + 3.7859 \times 10^{-6} \cdot (T/K)^2$; temp range 184–532 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

1107	(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
2479, 1564	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1082	(calculated-QSAR, Nirmalakhandan & Speece 1988)
978	(computed value, Yaws et al. 1991)
1192	(γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

1.90	(calculated-π const., Hansch et al. 1968)
2.14	(recommended, Hansch et al. 1995)
1.80	(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $k = 3.86 \times 10^{-6}$ s^{-1} with estimated $t_{1/2} \sim 2.0$ d at pH 7 and 25°C (Mabey & Mill 1978)

$k = 1.4 \times 10^{-2}$ h^{-1} at pH 7 and 25°C with estimated $t_{1/2} \sim 2.0$ d (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986);

rate constants at 25°C: $k = (379 \pm 41) \times 10^{-8}$ s^{-1} in distilled water at pH 3–11 for equal or more than 72% conversion (Mill et al. 1980; quoted, Haag & Mill 1988),

$k = (383 \pm 33) \times 10^{-8}$ s^{-1} in distilled water for 89% conversion, $k = (372 \pm 64) \times 10^{-8}$ s^{-1} in sediment-extracted water for 87% conversion, and $k = (420 \pm 80) \times 10^{-8}$ s^{-1} in sediment pores at pH 7.3 for 88% conversion (Haag & Mill 1988).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4$–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: estimated $t_{1/2} \sim 2.0$ d at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

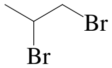
Ground water:

Sediment: $t_{1/2} = 2.1$ d, based on neutral and base-catalyzed hydrolysis studies at 25°C in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil:

Biota:

5.1.2.8 1,2-Dibromopropane



Common Name: 1,2-Dibromopropane
Synonym: propylene bromide, propylene dibromide
Chemical Name: 1,2-dibromopropane
CAS Registry No: 78-75-1
Molecular Formula:$C_3H_6Br_2$, $CH_3CHBrCH_2Br$
Molecular Weight: 201.888
Melting Point (°C):
  –55.49 (Lide 2003)
Boiling Point (°C):
  141.0 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.93268, 1.92344 (20°C, 25°C, Dreisbach 1959)
  1.9324, 1.9241 (20°C, 25°C, Dreisbach 1961)
  1.9324 (Horvath 1982; Weast 1982–83)
Molar Volume (cm^3/mol):
  104.5 (20°C, calculated-density)
  120.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  42.43, 35.52 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  8.937 (calculated, Dreisbach 1959; quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  1430 (measured by Dow Chemical, Dreisbach 1955–1961)
  1463 (Hine & Mookerjee 1975)
  1428 (recommended, Horvath 1982)
  2000 (Dean 1985)
  2986 (calculated-fragment const., Wakita et al. 1986)
  1919 (predicted-MCI χ and polarizability, Nirmalakhandan & Speece 1988)
  1420 (calculated-AI, Okouchi et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  2000 (37.3°C, Kahlbaum & Arndt 1898)
  1036 (Antoine eq. regression, temp range –7.0 to 141.6°C, Stull 1947)
  1071 (calculated-Antoine eq., Dreisbach 1959)
  $\log (P/mmHg) = 6.89105 - 1419.6/(212.0 + t/°C)$; temp range 50–210°C (Antoine eq. for liquid state, Dreisbach 1959)
  688 (calculated by formula, Dreisbach 1961)
  $\log (P/mmHg) = 7.34875 - 1572.7/(212.0 + t/°C)$; temp range 56–183°C (Antoine eq. for liquid state, Dreisbach 1961)
  $\log (P/mmHg) = [-0.2185 \times 9801.9/(T/K)] + 8.073203$; temp range –7.0 to 141.6°C (Antoine eq., Weast 1972–73)
  $\log (P/mmHg) = 7.30398 - 1644.4/(232.0 + t/°C)$; temp range 0–50°C (Antoine eq., Dean 1985, 1992)
  $\log (P/mmHg) = 6.89105 - 1419.6/(212.0 + t/°C)$; temp range 50–250°C (Antoine eq., Dean 1985, 1992)
  1072 (quoted from Dreisbach 1959, 1961, Riddick et al. 1986)
  $\log (P/kPa) = 6.01595 - 1419.6/(212.0 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
  $\log (P_L/kPa) = 6.47365 - 1572.7/(-61.15 + T/K)$; temp range 329–456 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.00898 – 1409.6/(–62.856 + T/K); temp range 312–403 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):

94.2	(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
21.1, 164	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
226.1	(calculated-QSAR, Nirmalakhandan & Speece 1988)
150	(computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.54	(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

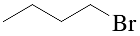
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Hydrolysis: rate constant k = (2.5 ± 0.5) × 10^{-8} s^{-1} in water at 25°C and pH 7 with $t_{1/2}$ ~ 320 d (Vogel & Reinhard 1986).

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

5.1.2.9 1-Bromobutane (*n*-Butyl bromide)



Common Name: 1-Bromobutane
Synonym: *n*-butyl bromide, monobromobutane
Chemical Name: 1-bromobutane, *n*-butyl bromide, monobromobutane
CAS Registry No: 109-65-9
Molecular Formula: C_4H_9Br, $CH_3CH_2CH_2CH_2Br$
Molecular Weight: 137.02
Melting Point (°C):
–112.6 (Lide 2003)
Boiling Point (°C):
101.6 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)
Density (g/cm^3 at 20°C):
1.2758, 1.2687 (20°C, 25°C, Dreisbach 1961; Horvath 1982; Riddick et al. 1986)
Molar Volume (cm^3/mol):
107.9 (20°C, calculated-density)
119.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
38.83, 31.85 (25°C, normal bp, Dreisbach 1961)
36.60, 31.85 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
6.694 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
580 (16°C, volumetric method, Fühner 1924)
608 (30°C, shake flask-interferometer, Gross & Saylor 1931)
598 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
254 (shake flask-volumetric method, Booth & Everson 1948)
509 (exptl., Korenman et al. 1971)
600 (selected exptl., Horvath 1982)
869 (generator column-GC, Tewari et al. 1982)
601 (calculated-UNIFAC activity coeff., Arbuckle 1986)
608 (30°C, quoted, Riddick et al. 1986)
680, 868, 871, 608 (16, 25, 25, 30°C, reported values, IUPAC-NIST Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
10972 (20°C, manometry, measured range 20–70°C, Smyth & Engel 1929)
5333 (24.8°C, summary of literature data, measured range –33.0 to 101.6°C, Stull 1947)
5502 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 6.92254 – 1298.608/(219.70 + t/°C); temp range 19–141°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.92254 – 1298.608/(219.70 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
log (P/mmHg) = [–0.2185 × 8789.1/(T/K)] + 8.028836; temp range –33.0 to 101.6°C (Antoine eq., Weast 1972–73)
5502 (selected, Riddick et al. 1986)
log (P/kPa) = 6.04744 – 1298.608/(219.70 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
5502 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.04744 – 1298.608/(–53.45 + T/K); temp range 273–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.1388 – 1349.142/(–48.003 + T/K); temp range 338–373 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/mmHg) = 74.7061 – 4.0663 × 10^3/(T/K) – 25.61·log (T/K) + 1.3166 × 10^{-2}·(T/K) + 1.421 × 10^{-13}·$(T/K)^2$; temp range 161–577 K (vapor pressure eq., Yaws 1994)
5506 (static method-manometer, measured range 278.15–323.15 K, Garriga et al. 2002)
ln (P/kPa) = 14.12331 – 3088.751/[(T/K) – 49.418]; temp range 278.15–323.15 K (static method, Garriga et al. 2002)

Henry's Law Constant (Pa m^3/mol at 25° C):

1242	(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
1600, 2313	(calculated-group contribution method, calculated-bond contribution Hine & Mookerjee 1975)
964.4	(calculated-QSAR, Nirmalakhandan & Speece 1988)
1223	(computed value, Yaws et al. 1991)
1215	(γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

2.75	(generator column-GC, DeVoe et al. 1981; Wasik et al. 1981; Tewari et al. 1982)
2.75	(generator column-HPLC, DeVoe et al. 1981)
2.79	(estimated-activity coefficients, Wasik et al. 1981)
2.64	(estimated-activity coefficients, Schantz & Martire 1987)
2.75	(recommended, Sangster 1989)
2.75	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

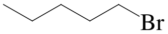
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976).

5.1.2.10 1-Bromopentane (*n*-Amyl bromide)



Common Name: 1-Bromopentane
Synonym: *n*-amyl bromide, monobromopentane, pentyl bromide
Chemical Name: *n*-amyl bromide, 1-bromopentane, monobromopentane, pentyl bromide
CAS Registry No: 110-53-2
Molecular Formula: $C_5H_{11}Br$, $CH_3CH_2CH_2CH_2CH_2Br$
Molecular Weight: 151.045
Melting Point (°C):
  –88.0 (Lide 2003)
Boiling Point (°C):
  129.8 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.2182, 1.2119 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm^3/mol):
  124.0 (20°C, calculated- density; Stephenson & Malanowski 1987)
  141.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  41.78, 34.49 (25°C, at normal bp, Dreisbach 1961)
  41.43, 34.49 (25°, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  11.46 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  127 (generator column-GC, Tewari et al. 1982)
  141 (calculated-UNIFAC activity coeff., Arbuckle 1986)
  127 (selected, Riddick et al. 1986)
  127 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  1754 (calculated by formula, Dreisbach 1961)
  $\log (P/mmHg) = 6.95580 – 1401.634/(214.38 + t/°C)$; temp range 41–171°C (Antoine eq. for liquid state, Dreisbach 1961)
  $\log (P/mmHg) = 6.95580 – 1401.634/(214.38 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
  1680 (quoted, Riddick et al. 1986)
  $\log (P/kPa) = 6.08070 – 11401.634/(214.38 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
  1680 (interpolated-Antoine eq., Malanowski 1987)
  $\log (P_L/kPa) = 6.0807 – 1401.634/(–58.77 + T/K)$; temp range 293–443 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
  2005 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
  3.37 (generator column-GC, DeVoe et al. 1981; Tewari et al. 1982)
  3.37 (generator column-HPLC, DeVoe et al. 1981)
  3.49 (generator column-GC, Wasik et al. 1981)
  3.32 (estimated-measured activity coefficients, Schantz & Martire 1987)
  3.37 (recommended, Sangster 1989)
  3.37 (calculated-UNIFAC activity coeff., Dallos et al. 1993)

3.37 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

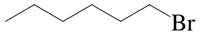
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h for the reaction with OH radicals in air (USEPA 1974; quoted, Darnall et al. 1976).

5.1.2.11 1-Bromohexane



Common Name: 1-Bromohexane
Synonym: *n*-hexyl bromide
Chemical Name: 1-bromohexane
CAS Registry No: 111-25-1
Molecular Formula: $C_6H_{13}Br$; CH3(CH2)4CH2Br
Molecular Weight: 165.071
Melting Point (°C):
–83.7 (Lide 2003)
Boiling Point (°C):
155.3 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3):
1.1744, 1.1667 (20°C, 25°C, Dreisbach 1961)
1.1744 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
140.6 (20°C, calculated-density, Stephenson & Malanowski 1987)
163.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
46.77, 37.07 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
25.75 (generator column-GC/FID, Tewari et al. 1982)
25.8 (tentative value, IUPAC-NIST Solubility Data Series, Hovrath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
520 (calculated-Antoine eq., Dreisbach 1961)
$\log (P/\text{mmHg}) = 7.0023 - 1503.52/(209.5 + t/°C)$; temp range 63–202°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/\text{mmHg}) = 7.0023 - 1503.52/(209.5 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
$\log (P_L/\text{kPa}) = 6.1272 - 1503.52/(T/K - 63.65)$; temp range 333–456 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
3.80 (generator column-GC, Tewari et al. 1982)
4.58 (HPLC-RT correlation, Burkhard et al. 1985)
3.80; 3.804 (generator column-GC; calculated-activity coeff. γ, Schantz & Martire 1987)
3.80 (recommended, Sangster 1989, 1993; Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

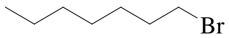
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

5.1.2.12 1-Bromoheptane



Common Name: 1-Bromoheptane
Synonym: heptyl bromide
Chemical Name: 1-bromoheptane
CAS Registry No: 629-04-9
Molecular Formula: $C_7H_{15}Br$
Molecular Weight: 179.098
Melting Point (°C):
–56.1 (Dreisbach 1961; Weast 1982–83; Lide 2003)
Boiling Point (°C):
178.9 (Dreisbach 1961; Weast 1982–83; Lide 2003)
Density (g/cm^3):
1.140, 1.1347 (20°C, 25°C, Dreisbach 1961)
1.140 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
157.1 (20°C, calculated-density, Stephenson & Malanowski 1987)
186.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
51.83, 39.59 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
6.68 (generator column-GC/GID, Tewari et al. 1982; Miller et al. 1985)
6.68 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
163 (calculated-Antoine eq., Dreisbach 1961)
$\log (P/mmHg) = 7.0582 - 1603.71/(205.0 + t/°C)$; temp range 82–228°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = 7.0582 - 1603.71/(205.0 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
$\log (P_L/kPa) = 6.1831 - 1603.71/(T/K - 68.15)$; temp range 333–483 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)
$\log (P/mmHg) = 43.3327 - 4.0389 \times 10^3/(T/K) - 12.105 \cdot \log (T/K) - 1.5959 \times 10^{-10} \cdot (T/K) + 3.0522 \times 10^{-6} \cdot (T/K)^2$; temp range 217–651 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
4.36 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
4.36; 4.44 (generator column-GC; calculated-activity coeff., Schantz & Mairtire 1987)
4.36 (recommended, Sangster 1989; 1994; Hansch et al. 1995)

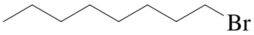
Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:

5.1.2.13 1-Bromooctane



Common Name: 1-Bromooctane
Synonym: octyl bromide
Chemical Name: 1-bromooctane
CAS Registry No: 111-83-1
Molecular Formula: $C_8H_{17}Br$, $CH_3(CH_2)_6CH_2Br$
Molecular Weight: 193.125
Melting Point (°C):
–55 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
200.8 (Dreisbach 1961; Weast 1982–83; Lide 2003)
Density (g/cm^3):
1.1122, 1.1072 (20°C, 25°C, Dreisbach 1961)
1.1122 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
174.3 (20°C, calculated-density, Stephenson & Malanowski 1987)
208.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
56.92, 42.04 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section)
1.67 (generator column-GC/FID, Tewari et al. 1982; Miller et al. 1985)
1.67 (tentative value, IUPAC-NIST Solubility Data Series, Hovrath & Getzen 1999b)
1.72* (24.9°C, generator column-GC, measured range 1.1–40.1°C, Sarraute et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
50.66 (calculated-Antoine eq., Dreisbach 1961)
$\log (P/mmHg) = 7.1179 - 1701.61/(200.8 + t/°C)$; temp range 101–253°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = 7.1179 - 1701.61/(200.8 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
$\log (P_L/kPa) = 6.2428 - 1701.61/(T/K - 72.35)$; temp range 373–475 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
50.53* (24.9°C, calculated-Antoine eq. of Li & Rossini 1961, temp range 1.1–40.1°C, Sarraute et al. 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):
5699* (calculated-P/C, temp range 1.1–40.1°C, Sarraute et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
4.89 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
4.89; 5.09 (generator column-GC; correlated-activity coeff., Schantz & Martire 1987)
4.89 (recommended, Sangster 1989, 1994; Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

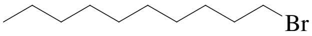
TABLE 5.1.2.13.1

Reported aqueous solubilities, vapor pressures and Henry's law constants of 1-bromooctane at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		

Aqueous solubility		Vapor pressure		Henry's law constant	
Sarraute et al. 2004		Sarraute et al. 2004		Sarraute et al. 2004	
generator column-GC		extrapolated -Antoine eq.#		calculated-P/C	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
1.10	2.66	1.10	6.567	1.10	478.8
5.0	2.22	5.0	9.431	5.0	809.4
5.2	2.414	5.2	9.606	5.2	777.4
9.9	1.76	9.9	14.69	9.9	1600
9.9	1.77	9.9	14.68	9.9	1600
14.9	1.82	14.9	22.60	14.9	2395
24.9	1.715	24.9	50.53	24.9	5699
29.9	2.18	29.9	73.61	29.9	6500
34.0	2.78	34.0	105.5	34.0	7350
40.0	3.65	40.0	150.1	40.0	7941
40.1	3.48	40.1	150.6	40.1	8360
		Antoine eq.			
		#see ref. Li & Rossini 1961			
		eq. 2	P/mmHg		
		A	7.1231		
		B	1369.20		
		C	204.4		
		pressure range 10–1500 torr mmHg			

5.1.2.14 1-Bromodecane



Common Name: 1-Bromodecane
Synonym: decyl bromide
Chemical Name: 1-bromohexane
CAS Registry No: 112-29-8
Molecular Formula: $C_{10}H_{21}Br$, $CH_3(CH_2)_8CH_2Br$
Molecular Weight: 221.178
Melting Point (°C):
–29.2 (Dreisbach 1961; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
240.6 (Dreisbach 1961; Weast 1982–83; Riddick et al. 1986; Lide 2003)
Density (g/cm^3):
1.0702, 1.0656 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
1.0702 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
206.7 (10°C, Stephenson & Malanowski 1987)
252.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
67.12, 46.66 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.33 (calculated-Antoine eq., Dreisbach 1961)
$\log (P/mmHg) = 7.2336 - 1888.67/(193.3 + t/°C)$; temp range 135–297°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = 7.2336 - 1888.67/(193.3 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
5.0 (quoted value from Dreisbach 1961, Riddick et al. 1986)
$\log (P/kPa) = 6.3585 - 1888.67/(193.3 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
$\log (P_L/kPa) = 6.3585 - 1888.67/(T/K - 79.85)$; temp range 383–570 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, log K_{OW}:
6.43 (HPLC-RT correlation, McDuffie 1981)
6.35, 5.84 (HPLC-RT correlation; calculated-CLOGP, Burkhard et al. 1985)
6.43 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

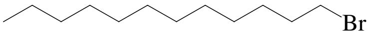
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

5.1.2.15 1-Bromododecane



Common Name: 1-Bromododecane
Synonym: lauryl bromide
Chemical Name: 1-bromododecane
CAS Registry No: 143-15-7
Molecular Formula: $C_{12}H_{25}Br$, $CH_3(CH_2)_{10}CH_2Br$
Molecular Weight: 249.231
Melting Point (°C):
  –9.5 (Dreisbach 1961; Weast 1982–83; Lide 2003)
Boiling Point (°C):
  276 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3):
  1.0399, 1.0355 (20°C, 25°C, Dreisbach 1961)
  1.0399 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
  240.1 (20°C, Stephenson & Malanowski 1987)
  297.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  77.38, 50.91 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  log (P/mmHg) = 7.3390 – 2061.93/(186.6 + t/°C); temp range 165–237°C (Antoine eq. for liquid state, Dreisbach 1961)
  log (P/mmHg) = 7.3390 – 2061.93/(186.6 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini. 1961)
  log (P/kPa) = 6.4639 – 2061.93/(T/K – 86.55); temp range 411–610 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
  6.98; 6.90 (HPLC-RT correlation; calculated-CLOPG, Burkhard et al. 1985)

Octanol/Air Partition Coefficient, log K_{OA}:

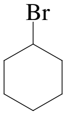
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

5.1.2.16 Bromocyclohexane



Common Name: Bromocyclohexane
Synonym: cyclohexyl bromide
Chemical Name: bromocyclohexane
CAS Registry No: 108-85-0
Molecular Formula: $C_6H_{11}Br$
Molecular Weight: 163.055
Melting Point (°C):
  –56.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
  166.2 (Weast 1982–83; Lide 2003)
Density (g/cm^3):
  1.33585, 1.32976 (20°C, 25°C, Dreisbach 1955)
  1.3359 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
  122.06, 122.6 (20°C, 25°C, calculated-density)
  141.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  37.59, 44.80 (normal bp, 25°C, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  8.70 (Dreisbach 1955)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  421 (calculated by formula, Dreisbach 1955)
  $\log (P/\text{mmHg}) = 6.97980 - 1572.19/(217.38 + t/°C)$; temp range 68–260°C (Antoine eq. for liquid state, Dreisbach 1955)
  $\log P/\text{mmHg} = 6.97980 - 1572.19/(t/°C + 217.38)$; temp range 68–200°C (Antoine eq., Dean 1992)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
  3.20 (shake flask-GC, Canton & Wagman 1983)
  3.20 (recommended, Sangster 1993)
  3.20 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

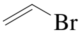
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

5.1.2.17 Vinyl bromide



Common Name: Vinyl bromide
Synonym: bromoethene, bromoethylene, ethylene bromide
Chemical Name: bromoethene
CAS Registry No: 593-60-2
Molecular Formula: C_2H_3Br, $CH_2 = CHBr$
Molecular Weight: 106.949
Melting Point (°C):
–139.54 (Dreisbach 1959; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
15.80 (Dreisbach 1959; Dean 1985; Riddick et al. 1986: Lide 2003)
Density (g/cm^3 at 20°C):
1.4933, 1.4738(20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
1.4930 (Dean 1985)
Molar Volume (cm^3/mol):
71.6 (20°C, calculated-density)
67.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
22.60, 23.45 (25°C, bp, Dreisbach 1959; Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
5.121 (Dreisbach 1959; Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4310 (30°C, shake flask-interferometry, Saylor & Gross 1931)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
101325 (15.8°C, summary of literature data, temp range –95.4–15.8°C, Stull 1947)
137700 (calculated-Antoine eq., Dreisbach 1959)
$\log (P/mmHg) = 6.66715 - 953.4/(236.0 + t/°C)$; temp range –60 to 60°C (Antoine eq. for liquid state, Dreisbach 1959)
145350 (extrapolated-Antoine eq., Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 6076.9/(T/K)] + 7.490979$; temp range –95.4 to 15.8°C (Antoine eq., Weast 1972–73)
144330, 139840 (calculated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 7.03256 - 1494.17/(281.722 + t/°C)$; temp range –66–11.9°C (Antoine eq. derived from exptl data of Mehl 1934, Boublik et al. 1984)
$\log (P/kPa) = 6.08611 - 1083.017/(249.845 + t/°C)$; temp range –87.5–16.0°C (Antoine eq. derived from exptl data of Guyer et al. 1937, Boublik et al. 1984)
137700 (selected lit. value, Riddick et al. 1986)
$\log (P/kPa) = 5.79205 - 953.4/(236.0 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
140480 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.03266 - 1014.0/(-37.15 + T/K)$; temp range 224–319 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = -10.9281 - 1.1619 \times 10^3/(T/K) + 9.3115\cdot\log (T/K) - 2.2655 \times 10^{-2}\cdot(T/K) - 4.531 \times 10^{-5}\cdot(T/K)^2$; temp range 135–473 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

1.57	(shake flask, Log P Database, Hansch & Leo 1987; recommended, Hansch et al. 1995)
1.57	(recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 6.81 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 25.4°C (Perry et al. 1977)

k_{OH}(calc) = 6.6×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 6.81×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1985)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{½}$ = 672–4320 h, based on aqueous screening test data for vinyl chloride (Heffgott et al. 1977; Freitag et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 2880–17280 h, based on estimated unacclimated aqueous aerobic half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 0.24–2.4 h from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

$t_{½}$ = 9.4–94 h, based on measured rate constant for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{½}$ = 1344–69000 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991) and an estimated half-life for anaerobic biodegradation of vinyl chloride from a ground water field study of chlorinated ethenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

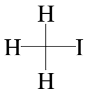
Sediment:

Soil: $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

5.1.3 IODOALKANES

5.1.3.1 Iodomethane (Methyl iodide)



Common Name: Methyl iodide
Synonym: iodomethane, monoiodomethane
Chemical Name: methyl iodide
CAS Registry No: 74-88-4
Molecular Formula: CH_3I
Molecular Weight: 141.949
Melting Point (°C):
–66.4 (Lide 2003)
Boiling Point (°C):
42.43 (Lide 2003)
Density (g/cm^3 at 20°C):
2.2790, 2.265 (20°C, 25°C, Dreisbach 1961)
2.2792, 2.265 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
62.28 (20°C, calculated-density)
62.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
27.97, 27.338 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
14190* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
13630 (20°C, Merckel 1937)
14200 (Seidell 1940; Seidell 1941)
log [C/(mol/L)] = –110.278 + 37.621·log (T/K) + 4823/(T/K); temp range 278.16–322.91 K (Glew & Moelwyn-Hughes 1953)
13900* (recommended, temp range 0–40°C, Horvath 1982)
14000 (20°C, Verschueren 1983; Riddick et al. 1986)
14000 (Dean 1985)

Vapor Pressure (Pa at 25°C, or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
44180, 64440(20°C, 30°C, Rex 1906)
75860* (34.4°C, temp range 0.10–34.4°C, Thompson & Linnett 1936)
53329* (25.3°C, summary of literature data, temp range –55.0 to 25.3°C, Stull 1947)
log (P/mmHg) = 22.974 – 5.346·log (T/K) – 2132/(T/K); temp range 278.16–322.91 K (Glew & Moelwyn-Hughes 1953)
54120 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.87991 – 1093.235/(230.94 + t/°C); temp range –29 to 76°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.87991 – 1093.235/(230.94 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
49704* (22.879°C, temp range –13.819 to 41.427°C, Boublik & Aim 1972; quoted, Boublik et al. 1984)
47750 (interpolated-Antoine eq., Weast 1972–73)

log (P/mmHg) = [–0.2185 × 6616.5/(T/K)] + 7.403018; temp range –55.0 to 254.8°C (Antoine eq., Weast 1972–73)
53980 (calculated-Antoine eq., Kudchadker et al. 1979)
log (P/mmHg) = 6.97241 – 1138.29/(t/°C + 235.774); temp range –14 to 42°C (Antoine eq., Kudchadker et al. 1979)
54120 (lit. average, Riddick et al. 1986)
log (P/kPa) = 6.09731 – 1138.29/(235.774 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
53960 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.10541 – 1142.67/(–36.87 + T/K); temp range 228–337 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = A6.17197 – 1240.17/(–17.887 + T/K); temp range 315–502 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = –20.3718 –1.2536 × 10^3/(T/K) + 13.645·log (T/K) –2.6955 × 10^{-2}·(T/K) + 1.6389 × 10^{-5}·$(T/K)^2$; temp range 207–528 K (vapor pressure eq., Yaws 1994)
54009 (selected summary of literature data, temp range 206.71–363.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
541*, 536 (exptl.-concn ratio, measured range 0–49°C, calculated-P/C, Glew & Moelwyn-Hughes 1953)
log {H/(mmHg·L/mol)} = 133.252 – 42.967·log (T/K) – 6955.2/(T/K); temp range 273.16–322.91 K (Glew & Moelwyn-Hughes 1953)
653* (29.43°C, concn ratio, measured range 29.43–40.34°C, Swain & Thornton 1962)
554.9 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
ln K_{AW} = 10.34 – 3541/(T/K); measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)
287 (computed value, Yaws et al. 1991)
159, 442 (0, 20°C, distilled water, headspace-GC, Elliott & Rowland 1993)
429 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
414 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K_{AW} = 4.059 – 1416/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
1.69 (19°C, shake flask, Collander 1951)
1.51 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)
1.51 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
2.16 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: photooxidation $t_{½}$ = 535–5348 h, based on a measured rate constant for the vapor phase reaction with hydroxyl radical in air (Garraway & Donovan 1979; quoted, Howard et al. 1991).
Hydrolysis: k = 7.28 × 10^{-8} s^{-1} at pH 7 (extrapolated to 25°C) with $t_{½}$ = 110 d (Mabey & Mill 1978).
Biodegradation: aqueous aerobic $t_{½}$ = 1168–672 h, based on estimated aerobic half-life (Howard et al. 1991); aqueous anaerobic $t_{½}$ = 672–2688 h, based on estimated aerobic half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); $t_{1/2}$ = 535–5348 h, based on a measured rate constant for the vapor phase reaction with hydroxyl radical in air (Garraway & Donovan 1979; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 168–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water:$t_{1/2}$ = 336–1344 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 168–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.3.1.1
Reported aqueous solubilities of iodomethane (methyl iodide) at various temperatures

$$S/(\text{wt\%}) = 1.53863 - 0.012169\cdot(t/°\text{C}) + 1.2714 \times 10^{-4}\cdot(t/°\text{C})^2 + 4.834 \times 10^{-6}\cdot(t/°\text{C})^3 \qquad (1)$$

Rex 1906		Horvath 1982	
volumetric method		summary of literature data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	15650	0	15386
10	14460	10	14345
20	14190	20	13848
30	14290	25	13848
		30	14185
		40	15646
		eq. 1	S/wt%

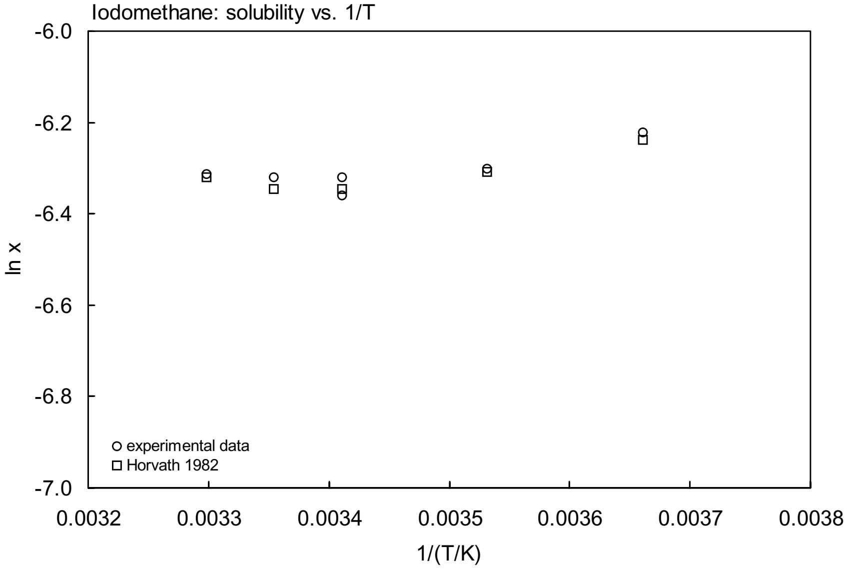


FIGURE 5.1.3.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for iodomethane.

TABLE 5.1.3.1.2
Reported vapor pressures of iodomethane (methyl iodide) at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K) (1)
log P = A – B/(C + t/°C) (2)
log P = A – B/(C + T/K) (3)
log P = A – B/(T/K) – C·log (T/K) (4)
ln P = A – B/(T/K) (1a)
ln P = A – B/(C + t/°C) (2a)

Thompson & Linnett 1936		Stull 1947		Boublik & Aim 1972	
		summary of literature data		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0.10	18932			–13.819	9306
4.30	22798	–55.5	666.6	–8.883	12046
11.70	31331	–45.8	1333	–5.101	14549
34.4	75860	–35.0	2666	–0.780	17921
		–24.2	5333	2.954	21314
		–16.9	7999	7.146	25780
		–7.0	13332	10.542	29923
		8.0	26664	14.567	35493
		25.3	53329	18.341	41470
		42.4	101325	22.879	49704
				28.342	61295
		mp/°C	–64.4	34.600	77125
				41.427	97913
				eq. 2	P/kPa
				A	6.11297
				B	1146.368
				C	236.677
				bp	42.431

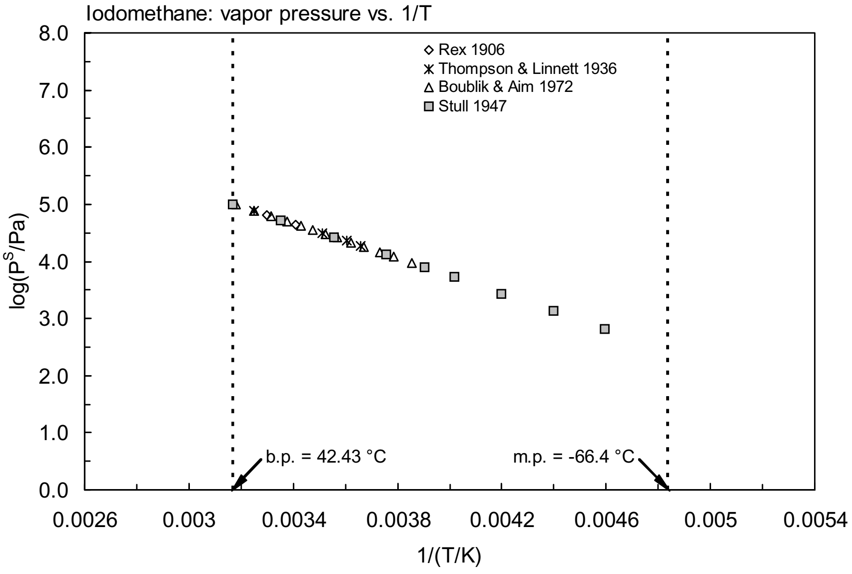


FIGURE 5.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for iodomethane.

TABLE 5.1.3.1.3
Reported Henry's law constants of iodomethane (methyl iodide) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1)

$\ln (1/K_{AW}) = A - B/(T/K)$ (2)

$\ln (k_H/atm) = A - B/(T/K)$ (3)

$\ln H = A - B/(T/K)$ (4)

$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

$\log H = A - B\cdot\log (T/K) - C/(T/K)$ (6)

$\log K_{AW} = A - B/(T/K)$ (1a)

$\log (1/K_{AW}) = A - B/(T/K)$ (2a)

Glew & Moelwyn-Hughes 1953		Swain & Thorton 1962		Elliot & Rowland 1993	
concentration ratio		concentration ratio		headspace-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
0	169.9	29.45	653	0	159
5.03	224.8	29.44	651	20	442
10.2	288.0	40.35	923		
15.12	364.0	40.34	913		
19.94	450.6				
24.92	541.2				
34.92	630.6				
39.86	738.6				
44.87	850.6				
49.75	1072				
25.0	536				
eq 6	P/(mmHg·L/mol)				
A	71.005				
B	21.656				
C	4043.9				

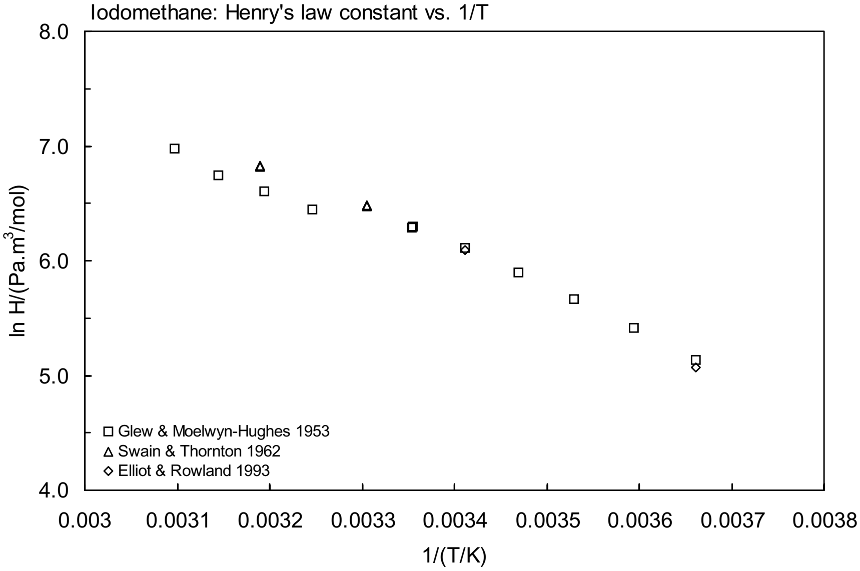
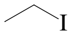


FIGURE 5.1.3.1.3 Logarithm of Henry's law constant versus reciprocal temperature for iodomethane.

5.1.3.2 Iodoethane (Ethyl iodide)



Common Name: Ethyl iodide
Synonym: iodoethane
Chemical Name: ethyl iodide, iodoethane,
CAS Registry No: 75-03-6
Molecular Formula: C_2H_5I, CH_3CH_2I
Molecular Weight: 155.965
Melting Point (°C):
–111.1 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
72.30 (Rex 1906; Dreisbach 1961; Horvath 1982; Riddick et al. 1986; Lide 2003)
Density (g/cm^3 at 20°C):
1.9358, 1.9245 (20°C, 25°C, Dreisbach 1961)
1.9357, 1.9244 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
80.6 (20°C, calculated from density)
85.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
31.93, 29.77 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
4030* (20°C, volumetric method, measured range 0–30°C, Rex 1906;)
3910 (22.5°C, volumetric method, Führer 1924)
4040 (30°C, shake flask-interferometry, Gross & Saylor 1931)
4040 (30°C, shake flask, Van Arkel & Vles 1936)
3915 (20°C, Merckel 1937)
3918 (Seidell 1940,1941; quoted, Deno & Berkheimer 1960; Hansch et al. 1968; Hine & Mookerjee 1975)
3915 (22.5°C, Saracco & Spaccamela Marchetti 1958)
3920 (20°C, exptl., Korenman et al. 1971)
4041* (summary of literature data temp range 0–30°C, Horvath 1982)
3880 (30°C, selected, Riddick et al. 1986)
4000* (tentative value, temp range 0–30°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = $8.5757 - 5.5568 \times 10^{-2}\cdot(T/K) + 9.43918 \times 10^{-5}\cdot(T/K)^2$, temp range 273–303 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
14280, 22150 (20°C, 30°C, Rex 1906)
21678* (30°C, manometry, measured range 30–60°C, Smyth & Engel 1929)
14612* (20°C, temp range –19.36 to 20.4°C, Milazzo 1944)
13332* (18°C, summary of literature data, temp range –54.4 to 72.4°C, Stull 1947)
18160 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = $6.83198 - 1175.709/(225.26 + t/°C)$; temp range –6 to 109°C, (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = $6.83198 - 1175.709/(225.26 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
log (P/mmHg) = $[-0.2185 \times 6843.1/(T/K)] + 7.635277$; temp range –74.3 to 229.5°C (Antoine eq., Weast 1972–73)

log (P/kPa) = 7.12695 – 1823.148/(285.30 + t/°C); temp range –19.36 to 20.4°C (Antoine eq. derived from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.06765 – 1222.410/(228.368 + t/°C), temp range 30–60°C (Antoine eq. derived from reported experimental data, Boublik et al. 1984)
log (P/mmHg) = 6.959 – 1232.0/(229.0 + t/°C); temp range 30–60°C (Antoine eq., Dean 1985, 1992)
log (P/kPa) = 5.95688 – 1175.709/(225.26 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
18430 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.95686 – 1175.709/(–47.89 + T/K); temp range 249–369 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 31.4422 – 2.5719×10^3/(T/K) – 8.4867·log (T/K) – 9.0736×10^{-11}·(T/K) + 3.571×10^{-6}·$(T/K)^2$; temp range 162–561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

732	(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
840	(calculated-QSAR, Nirmalakhandan & Speece 1988)
545	(computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.00	(shake flask-GC, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)
2.00	(recommended, Sangster 1989, 1993)
2.00	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

2.59	(calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Hydrolysis: rate constant k = 1.62×10^{-7} s^{-1} with $t_{½}$ = 49 d at 25°C and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:
Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).
Surface water: $t_{½}$ = 49 d at 25°C and pH 7 (Mabey & Mill 1978)
Ground water:
Sediment:
Soil:
Biota:

TABLE 5.1.3.2.1
Reported aqueous solubilities of 1-iodoethane at various temperatures

$$S/(\text{wt\%}) = 0.4391 - 3.24498 \times 10^{-3}\cdot(t/°\text{C}) + 4.49991 \times 10^{-5}\cdot(t/°\text{C})^2 + 1.15001 \times 10^{-6}\cdot(t/°\text{C})^3 \quad (1)$$

$$S/(\text{wt\%}) = 8.5757 - 5.5568 \times 10^{-2}\cdot(T/\text{K}) + 9.43918 \times 10^{-4}\cdot(T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999a	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
0	4410	0	4391	0	4400
10	4140	10	4123	5	4220
20	4030	20	4014	10	4090
30	4150	25	4041	15	4010
		30	4133	20	3980
				25	4000
		eq. 1	S/wt%	30	4050
				eq. 2	S/wt%
				temp range 273–303 K	

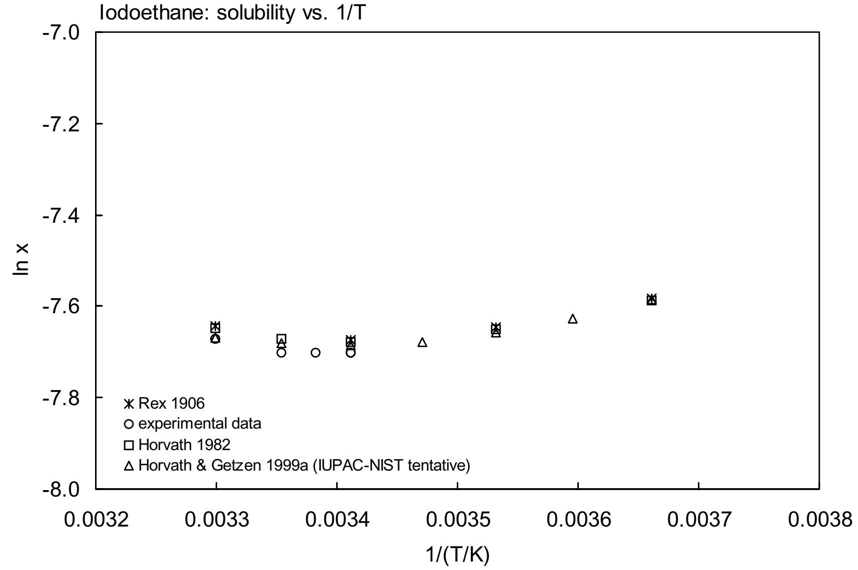


FIGURE 5.1.3.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for iodoethane.

TABLE 5.1.3.2.2
Reported vapor pressures of iodoethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Smyth & Engel 1929		Milazzo 1944		Stull 1947	
Manometry				summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30.0	21678	−19.36	1867	−54.4	133.3
40.0	32637	0.040	5533	−34.3	666.6
50.0	47329	9.34	8666	−24.3	1333
60.0	67448	10.4	9066	−13.1	2666
		20.4	14612	−0.90	5333
				7.2	7999
				18.0	13332
				34.1	26664
				52.3	53329
				72.4	101325
				mp/°C	−105

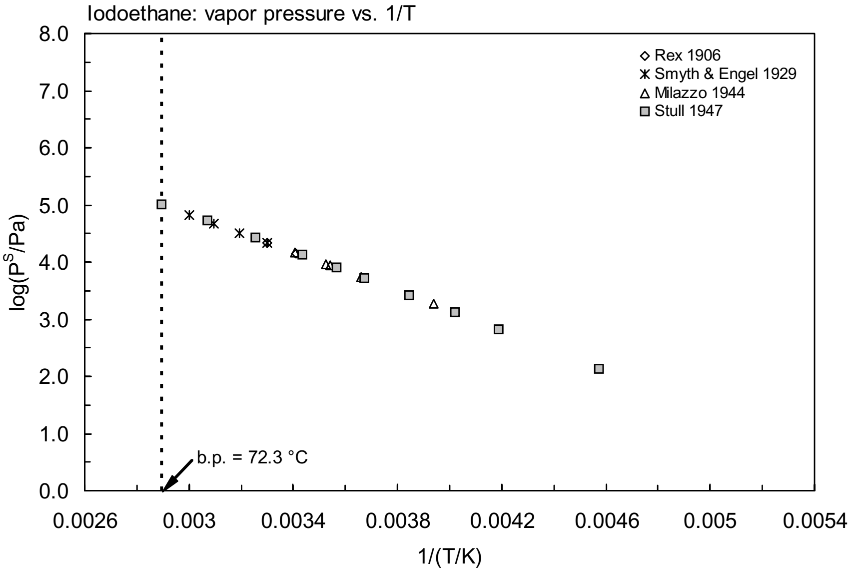
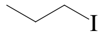


FIGURE 5.1.3.2.2 Logarithm of vapor pressure versus reciprocal temperature for iodoethane.

5.1.3.3 1-Iodopropane



Common Name: 1-Iodopropane
Synonym: monoiodopropane, *n*-propyl iodide, propyl iodide
Chemical Name: 1-iodopropane, monoiodopropane, *n*-propyl iodide, propyl iodide
CAS Registry No: 107-08-4
Molecular Formula: C_3H_7I, $CH_3CH_2CH_2I$
Molecular Weight: 169.992
Melting Point (°C):
–101.3 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
102.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.7489, 1.7394 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm^3/mol):
97.2 (20°C, calculated-density)
107.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
45.98, 31.70 (25°C, bp, Dreisbach 1961)
36.25 (25°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
1070* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
867 (20°C, volumetric method, Fühner 1924)
1040 (30°C, shake flask-interferometer, Gross & Saylor 1931)
1037 (30°C, shake flask, Van Arkel & Vles 1936)
1073 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
872 (Seidell 1941)
1110 (calculated-K_{OW}, Hansch et al. 1968)
1070, 1060 (23.5°C, elution chromatography, Schwarz 1980)
1051* (summary of literature data, temp range 0–30°C, Horvath 1982)
1000 (Dean 1985)
1040 (30°C, quoted, Riddick et al. 1986)
1010* (tentative value, temp range 0–30°C, IUPAC-NIST Series, Horvath & Getzen 1999b)
$S/(wt\%) = 3.4659 - 0.023046\cdot(T/K) + 3.94424 \times 10^{-5}\cdot(T/K)^2$, temp range 273–303 K (equation derived from literature data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4679, 7305 (20°C, 30°C, volumetric method Rex, 1906)
5333 (23.6°C, summary of literature, data temp range –36.0 to 102.5°C, Stull 1947)
5745 (calculated-Antoine eq., Dreisbach 1961)
$\log (P/mmHg) = 6.81603 - 1267.062/(219.53 + t/°C)$; temp range 18–143°C (Antoine eq. for liquid state, Dreisbach 1961)
$\log (P/mmHg) = 6.81603 - 1267.062/(219.53 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
$\log (P/mmHg) = [-0.2185 \times 8467.1/(T/K)] + 7.824521$; temp range –36.0 to 102.5°C (Antoine eq., Weast 1972–73)
5745 (quoted lit. average, Riddick et al. 1986)
$\log (P/kPa) = 5.94053 - 1267.062/(219.53 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

5745 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.6036 - 1160.5/(-59.55 + T/\text{K})$; temp range 171–271 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.94093 - 1267.062/(-52.62 + T/\text{K})$; temp range 271–402 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 1.2733 - 2.0214 \times 10^3/(T/\text{K}) + 4.1138\cdot\log(T/\text{K}) - 1.2477 \times 10^{-2}\cdot(T/\text{K}) + 7.678 \times 10^{-6}\cdot(T/\text{K})^2$; temp range 172–593 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

921	(calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
1033, 1082	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1057	(calculated-QSAR, Nirmalakhandan & Speece 1988)
844	(computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.50	(calculated-π const., Hansch et al. 1968)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 5.1.3.3.1
Reported aqueous solubilities of 1-iodopropane at various temperatures

$$S/(\text{wt}\%) = 0.1139 - 4.86669 \times 10^{-4}\cdot(t/°\text{C}) + 1.25003 \times 10^{-5}\cdot(t/°\text{C})^2 - 2.8334 \times 10^{-7}\cdot(t/°\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 3.4659 - 0.023046\cdot(T/\text{K}) + 3.94424 \times 10^{-5}\cdot(T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999b	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	1140	0	1139	0	1140
10	1030	10	1100	5	1070
20	1070	20	1069	10	1030
30	1030	25	1051	15	1000
		30	1029	20	1000
				25	1010
		eq. 1	S/wt%	30	1040
				eq. 2	S/wt%
				temp range 273–303 K	

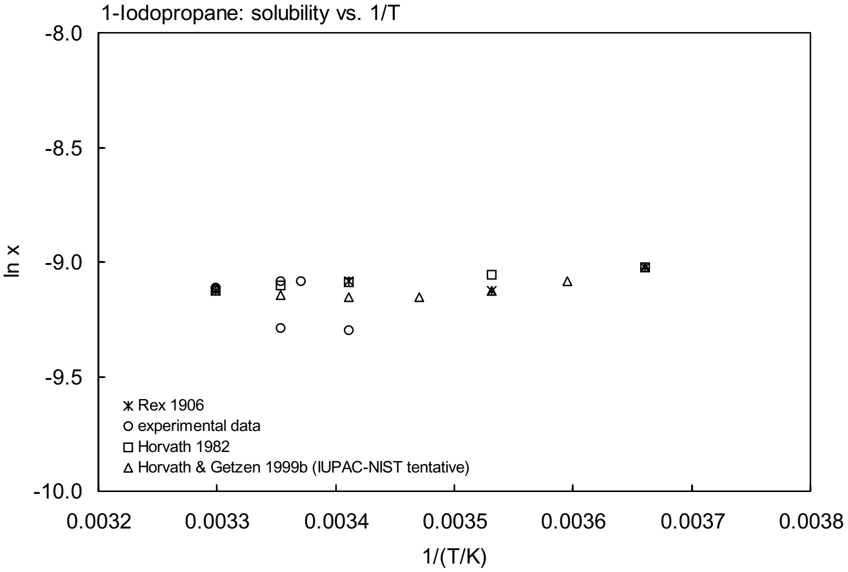
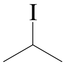


FIGURE 5.1.3.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1-iodopropane.

5.1.3.4 2-Iodopropane



Common Name: 2-Iodopropane
Synonym: isopropyl iodide
Chemical Name: 2-iodopropane, isopropyl iodide
CAS Registry No: 75-30-9
Molecular Formula: C_3H_7I, CH_3CHICH_3
Molecular Weight: 169.992
Melting Point (°C):
–90.0 (Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
89.50 (Riddick et al. 1986; Lide 2003)
Density (g/cm^3 at 20°C):
1.7042, 1.6946 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
99.8, 100.3 (20°C, 25°C, calculated-density)
107.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
34.06 (25°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1670, 1430, 1400, 1340 (0, 10, 20, 30°C, volumetric method, Rex 1906)
1343 (30°C, shake flask, Van Arkel & Vles 1936)
1667, 1428, 1398, 1387, 1338 (0, 10, 20, 25, 30°C, summary of literature data, Horvath 1982)
$S/(\text{wt}\%) = 0.1667 - 4.23167 \times 10^{-3} \cdot t/°C + 0.000224 \cdot (t/°C)^2 - 3.98334 \times 10^{-6} \cdot (t/°C)^3$ (Horvath 1982)
1400 (20°C, selected, Riddick et al. 1986)
1670, 1430, 1400, 1340 (0, 10, 20, 30°C, reported exptl data of Rex 1906, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
7518, 11780 (20°C, 30°C, Rex 1906)
7999 (21.6°C, summary of literature data, temp range –43.3 to 89.5°C, Stull 1947)
$\log (P/\text{mmHg}) = [-0.2185 \times 8243.4/(T/K)] + 7.873828$; temp range –43.3 to 89.5°C (Antoine eq., Weast 1972–73)
5700 (selected, Riddick et al. 1986)
$\log (P/\text{kPa}) = 6.87492 - 1765.15/(T/K)$; temp range not specified (Antoine eq., Riddick et al. 1986)
9360 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.2763 - 1414.85/(-31.45 + T/K)$; temp range 261–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 5.2724 - 989.55/(-69.18 + T/K)$; temp range 173–262 K (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = 33.2023 - 2.7569 \times 10^3/(T/K) - 9.0585 \cdot \log (T/K) - 1.2099 \times 10^{-10} \cdot (T/K) + 3.5044 \times 10^{-6} \cdot (T/K)^2$; temp range 183–578 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
1133 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
2479, 1982 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1840 (calculated-QSAR, Nirmalakhandan & Speece 1988)
903 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

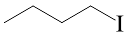
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Hydrolysis: rate constant k = 2.77×10^{-6} s^{-1} with $t_{½}$ = 2.9 d at 25°C and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:
Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).
Surface water: $t_{½}$ = 2.9 d at 25°C and pH 7 based on hydrolysis rate constant (Mabey & Mill 1978)
Ground water:
Sediment:
Soil:
Biota:

5.1.3.5 1-Iodobutane



Common Name: 1-Iodobutane
Synonym: *n*-butyl iodide, monoiodobutane
Chemical Name: *n*-butyl iodide, 1-iodobutane, monoiodobutane
CAS Registry No: 542-69-8
Molecular Formula: C_4H_9I, $CH_3CH_2CH_2CH_2I$
Molecular Weight: 184.018
Melting Point (°C):
–103.0 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
130.53 (Dreisbach 1961; Riddick et al. 1986)
130.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.6154, 1.6072 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm^3/mol):
113.9, 114.5 (20°C, 25°C, calculated- density, Riddick et al. 1986)
129.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
40.63, 33.40 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
210 (17.5°C, volumetric method, Fühner 1924)
202 (20°C, Merckel 1937)
211 (Seidell 1940; quoted, Deno & Berkheimer 1960)
202 (Seidell 1941)
313 (Kakovsky 1957)
182 (selected exptl., Horvath 1982)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1848 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.82262 – 1358.860/(214.2 + t/°C); temp range 40–174°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.82262 – 1358.860/(214.20 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq., from correlation of selected lit. data, Li & Rossini 1961)
log (P/kPa) = 5.94752 – 1358.860/(214.20 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
1848 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.94752 – 1358.86/(–58.95 + T/K); temp range 292–431 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
1600 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
1426, 600 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1331 (calculated-QSAR, Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
3.00 (calculated-π const., Hansch et al. 1968)
2.51 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

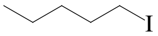
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976).

5.1.3.6 1-Iodopentane



Common Name: 1-Iodopentane
Synonym: pentyl iodide
Chemical Name: 1-iodopentane
CAS Registry No: 628-17-1
Molecular Formula: $C_5H_{11}I$, $CH_3(CH_2)_3CH_2I$
Molecular Weight: 198.045
Melting Point (°C):

–85.6	(Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

157	(Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987: Lide 2003)

Density (g/cm^3):

1.5061, 1.5088	(20°C, 25°C, Dreisbach 1961)
1.5161	(20°C, Weast 1982–83)

Molar Volume (cm^3/mol):

130.6	(20°C, calculated-density, Stephenson & Malanowski 1987)
151.7	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

43.33, 35.81	(25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

585	(calculated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.85172 – 1454.028/(209.17 + t/°C); temp range 61–204°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.85172 – 1454.028/(209.17 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
log P_L/kPa = 5.97662 – 1454.028/(–63.98 + T/K); temp range 312–413 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

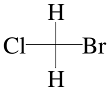
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

5.1.4 MIXED HALOGENATED HYDROCARBONS

5.1.4.1 Bromochloromethane



Common Name: Bromochloromethane
Synonym: chlorobromomethane, methylene bromochloride
Chemical Name: bromochloromethane, chlorobromomethane
CAS Registry No: 74-97-5
Molecular Formula: CH_2BrCl
Molecular Weight: 129.384
Melting Point (°C):
–87.9 (Lide 2003)
Boiling Point (°C):
68.0 (Lide 2003)
Density (g/cm^3 at 20°C):
1.9344 (Dreisbach 1959; Weast 1982–83; Riddick et al. 1986)
1.9229 (25°C, Dreisbach 1959)
Molar Volume (cm^3/mol):
66.89 (20°C, calculated-density)
73.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

15000	(O'Connell 1963)
9000	(Kirk-Othmer 1964, Irmann 1965, Dean 1985)
15000	(Jolls 1966)
14778	(at saturated pressure, recommended, Horvath 1982)
16690	(generator column-GC, Tewari et al. 1982)
38900	(calculated-UNIFAC activity coeff., Arbuckle 1986)
17000	(selected, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
18808 (24.06°C, ebulliometric method, measured range 15.72–68°C, McDonald et al. 1959)
$\log (P/mmHg) = 6.38587 - 895.556/(186.703 + t/°C)$; temp range 15.72–68.0°C (Antoine eq. from ebulliometric measurements, McDonald et al. 1959)
19620 (calculated-Antoine eq., Dreisbach 1959)
$\log (P/mmHg) = 6.86624 - 1132.3/(215.0 + t/°C)$; temp range –6 to 297°C (Antoine eq. for liquid state, Dreisbach 1959)
19520 (calculated-Antoine eq., Boublik et al. 1973)
$\log (P/mmHg) = 6.49606 - 942.267/(192.587 + t/°C)$; temp range 15.7–68°C (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1973)
19520 (calculated-Antoine eq., Kudchadker et al. 1979)
$\log (P/mmHg) = 6.41307 - 903.382/(187.594 + t/°C)$; temp range 16–68°C (Antoine eq., Kudchadker et al. 1979)
$\log (P/kPa) = 6.60056 - 932.609/(191.376 + t/°C)$; temp range 15.7–68°C (Antoine eq. from reported exptl. data of McDonald & Shrader 1959, Boublik et al. 1984)
19530 (calculated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 5.51146 - 891.345/(-86.965 + T/K)$; temp range 226–341 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 2.7704 – 2.0139 × 10^3/(T/K) + 3.7817·log (T/K) – 1.3241 × 10^{-2}·(T/K) + 8.1979 × 10^{-6}·$(T/K)^2$; temp range 185–557 K (vapor pressure eq., Yaws 1994)
19257 (selected summary of literature data, temp range 185.21–368.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
1.41 (generator column-GC, Tewari et al. 1982)
1.41 (recommended, Sangster 1993)
1.41 (recommended, Hansch et al. 1995)

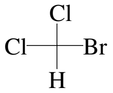
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
rate constant for the reaction with OH^-: k = (2.5 ± 0.3) × 10^{-6} M^{-1} s^{-1} was measured in 66.7% dioxane-water at 35.7°C (Hine et al. 1956; quoted, Roberts et al. 1992)
k_{OH} = 1.11 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} with atmospheric lifetime τ = 0.43 yr at 298 K, measured range 277–377 K (flash photolysis resonance fluorescence and discharge flow electron paramagnetic resonance, Orkin et al. 1997)
Hydrolysis: rate constant k = 1.2 × 10^{-10} s^{-1} with $t_{1/2}$ = 44 yr at pH 7 and 25°C (Mabey & Mill 1978)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976)
Atmospheric lifetime τ = 0.21 yr reduced from 0.43 yr due to reaction with OH with ocean removal (Orkin et al. 1997)
Surface water: hydrolysis rate constant k = 1.2 × 10^{-10} s^{-1} with $t_{1/2}$ = 44 yr at pH 7 and 25°C (Mabey & Mill 1978)

5.1.4.2 Bromodichloromethane



$CHCl_2Br$

Common Name: Bromodichloromethane
Synonym: dichlorobromomethane
Chemical Name: bromodichloromethane, dichlorobromomethane
CAS Registry No: 75-27-4
Molecular Formula: $CHBrCl_2$
Molecular Weight: 163.829
Melting Point (°C):
–57 (Lide 2003)
Boiling Point (°C):
90.0 (Weast 1977; Lide 2003)
Density (g/cm^3 at 20°C):
1.9710 (25°C, Verschueren 1983)
Molar Volume (cm^3/mol):
83.1 (20°C, calculated-density)
94.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4700 (22°C, Mabey et al. 1981)
2968 (30°C, headspace-GC, McNally & Grob 1984)
8880, 8668, 8506 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6665 (20°C, Dreisbach 1952;)
8555, 13440, 20444 (20, 30, 40°C, DIPPR compilation, Tse et al. 1992)

Henry's Law Constant (Pa m^3/mol at 25°C and reported temperature dependence equations):
244.2 (20°C, calculated-P/C, Mabey et al. 1982)
162 (20°C, batch air stripping-GC, Nicholson et al. 1984)
162, 152, 152 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)
$\ln [H/(\text{atm m}^3/\text{mol})] = 11.30 - 5210/(T/K)$; temp range 10–30°C (air stripping-GC measurements, Nicholson et al. 1984)
214.8 (gas stripping-GC, Warner et al. 1987)
243.1 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
243 (calculated-P/C, Mackay & Shiu 1990)
162, 263, 405 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
55.2, 106, 192 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
$\ln K_{AW} = 13.43 - 4678/(T/K)$; seawater of salinity of 30.4‰, temp range: 0–10°C (Moore et al. 1995)
185 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 6.143 - 2130/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)
347 (37°C, equilibrium headspace-GC, Batterman et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
1.88 (calculated as per Tute 1971, Callahan et al. 1979; Mills et al. 1982)
2.10 (Hansch & Leo 1979)
2.10 (calculated, Mabey et al. 1982)
2.00 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}

2.98; 2.97 (equilibrium headspace-GC; calculated-K_{OW}/K_{AW}, Batterman et al. 2002)

Bioconcentration Factor, log BCF:

1.544 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
0.72–1.37 (estimated as per Lyman et al. 1982, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

1.785 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.724–2.40 (estimated from S & K_{OW}, Swann et al. 1983; quoted, Howard 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization: typical $t_{½}$ ~35 h for a range of 33 min to 12 d was estimated from experimentally determined gas transfer rates (Kaczmar et al. 1984; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

calculated rate constants at 25°C: k << 360 M^{-1} h^{-1} for singlet oxygen and k = 0.2 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982).

Hydrolysis: first-order rate constant $k = 1.6 \times 10^{-10}$ s^{-1} at pH 7 and 25°C with a maximum $t_{½}$ = 137 yr (Mabey & Mill 1978; quoted, Mabey et al. 1982; Howard 1990).

Biodegradation:

Biotransformation: estimated rate constant $k = 1 \times 10^{-10}$ mL $cell^{-1}$ h^{-1} for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

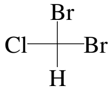
Half-Lives in the Environment:

Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (Darnall et al. 1976);

$t_{½}$ = 3.92 months, based on an estimated rate constant $k = 8.522 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} for the vapor phase reaction with hydroxyl radical (GEMS 1987; quoted, Howard 1990).

Surface water: hydrolysis rate constant $k = 1.6 \times 10^{-10}$ s^{-1} with $t_{½}$ = 137 yr at pH 7 and 25°C (Mabey & Mill 1978)

5.1.4.3 Dibromochloromethane



Common Name: Dibromochloromethane
Synonym: chlorodibromomethane
Chemical Name: dibromochloromethane, chlorodibromomethane
CAS Registry No: 124-48-1
Molecular Formula: $CHBr_2Cl$
Molecular Weight: 208.280
Melting Point (°C):
–22.0 (Dean 1985)
–20 (Lide 2003)
Boiling Point (°C):
119–120 (Weast 1977; Weast 1982–83)
120 (Lide 2003)
Density (g/cm^3 at 20°C):
2.451 (Weast 1982–83; Dean 1985)
Molar Volume (cm^3/mol):
84.98 (20°C, calculated-density)
97.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
4000 (calculated-K_{OW}, Mabey et al. 1982)
5814, 6000, 6102 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
10131 (20°C, extrapolated-Antoine eq., Mabey et al. 1982)
2000 (20°C, selected, Mills et al. 1982)
6667 (20°C, Warner et al. 1987)
2324, 3877, 6232 (20, 30, 40°C, DIPPR compilation, Tse et al. 1992)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
100 (20°C, calculated-P/C, Mabey et al. 1982)
88.2; 88.1, 85.1 (20°C, batch air stripping-GC; quoted lit. values, Nicholson et al. 1984)
86.1, 81.06, 78.02 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)
$\ln [H/(\text{atm m}^3/\text{mol})] = 10.70 - 5210/(T/K)$; temp range 10–30°C (air stripping-GC measurements, Nicholson et al. 1984)
80.4 (gas stripping-GC, Warner et al. 1987)
120* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 14.62 - 6373/(T/K)$; temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)
100 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
81.06, 142, 223 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
28.2, 56.3, 103 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
$\ln K_{AW} = 13.62 - 4914/(T/K)$; seawater of salinity of 30.4‰, temp range: 0–10°C (Moore et al. 1995)
85.3 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 6.296 - 2273/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)
218 (37°C, equilibrium headspace-GC, Batterman et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

2.09 (calculated as per Tute 1971, Callahan et al. 1979)
2.24 (Hansch & Leo 1979)
2.24 (calculated, Mabey et al. 1982)
2.16 (recommended, Sangster 1993)
2.04 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

3.59 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)
3.33; 3.31 (equilibrium headspace-GC; calculated-K_{OW}/K_{AW}, Batterman et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: calculated $t_{1/2}$ = 43 min to 16.6 d (using Langbein & Durum 1967 published O_2 re-aeration values) and $t_{1/2}$ = 45.9 h both from rivers and streams (Kaczmar et al. 1984).

Photolysis:

Oxidation: calculated rate constants at 25°C: k << 360 $M^{-1}\ h^{-1}$ for singlet oxygen and k = 0.5 $M^{-1}\ h^{-1}$ for peroxy radicals (Mabey et al. 1982);

photooxidation $t_{1/2}$ = 1025–10252 h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: rate constant k = $8.0 \times 10^{-11}\ s^{-1}$ with hydrolytic $t_{1/2}$ = 274 yr at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Howard et al. 1991);

k = $2.88 \times 10^{-8}\ h^{-1}$ at pH 7 and 25°C (analogy to chloroform as per Mabey & Mill 1978, Mabey et al. 1982).

Biodegradation: aqueous aerobic $t_{1/2}$ = 672–4320 h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 672–4320 h, based on unacclimated anaerobic screening test data (Bouwer & McCarty 1983; Bouwer et al. 1981; quoted, Howard et al. 1991).

Biotransformation: estimated rate constant k = 1.0×10^{-10} mL $cell^{-1}\ h^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); $t_{1/2}$ = 1025–10252 h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 274 yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{1/2}$ = 672–4320 h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2}$ = 336–4320 h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 672–4320 h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.4.3.1
Reported Henry's law constants of dibromochloromethane at various temperatures

Ashworth et al. 1988	
EPICS-GC	
t/°C	H/(Pa m^3/mol)
10	38.50
15	45.60
20	104.4
25	119.6
30	154.0
ln [H/(atm·m^3/mol)] = A – B/(T/K)	
A	14.62
B	6373

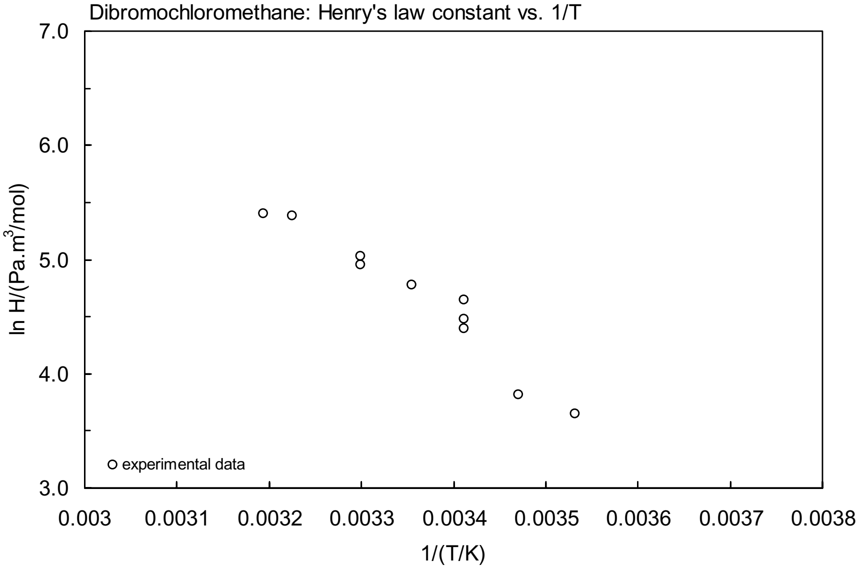
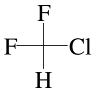


FIGURE 5.1.4.3.1 Logarithm of Henry's law constant versus reciprocal temperature for dibromochloromethane.

5.1.4.4 Chlorodifluoromethane (HCFC-22)



Common Name: Chlorodifluoromethane
Synonym: difluorochloromethane, Freon 22, CFC-22, CF-22
Chemical Name: chlorodifluoromethane
CAS Registry No: 75-45-6
Molecular Formula: $CHClF_2$
Molecular Weight: 86.469
Melting Point (°C):
–157.42 (Lide 2003)
Boiling Point (°C):
–40.7 (Lide 2003)
Density (g/cm^3 at 20°C):
1.2090 (21°C, Dean 1985)
1.1940 (25°C, Kirk-Othmer 1985)
1.2136, 1.1942 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
71.2 (20°C, calculated-density)
60.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
20.238 (bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
4.123 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:

Water Solubility (g/m^3 or mg/L at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):
2800, 2900 (quoted values, Irmann 1965)
3000 (DuPont 1966,1969; quoted, Horvath 1982; Riddick et al. 1986)
2930 (selected, Hine & Mookerjee 1975)
3000 (Weast 1976; quoted, Horvath 1982)
2899* (summary of literature data, temp range 0–60°C, Horvath 1982)
3000 (Dean 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
101325* (–40.8°C, summary of literature data, temp range –122.8 to –40.8°C, Stull 1947)
1083100 (calculated-Antoine eq., Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 5212.9/(T/K)] + 7.730042$; temp range –122.8 to 85.3°C (Antoine eq., Weast 1972–73)
$\log (P/mmHg) = 6.93892 - 808.919/(t/°C + 240.161)$; temp range –79 to –37°C (Antoine eq., Kudchadker et al. 1979)
1027400 (calculated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 6.0741 - 815.920/(241.369 + t/°C)$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
35120, 570500 (–61.26°C, 4.5°C, Riddick et al. 1986)
$\log (P/kPa) = 6.06382 - 808.919/(240.161 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
1043900 (Interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.33292 - 919.834/(-19.718 + T/K)$; temp range 170–233 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.19138 – 863.436/(–26.04 + T/K); temp range 230–275 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.35713 – 950.38/(–13.474 + T/K); temp range 275–327 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.13064 – 1490.048/(64.627 + T/K); temp range 324–366 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P/mmHg) = 40.3847 – 2.0731 × 10^3/(T/K) –12.317·log (T/K) – 2.5116 × 10^{-10}·(T/K) + 1.0498 × 10^{-5}·$(T/K)^2$; temp range 116–369 K (vapor pressure eq., Yaws 1994)
132020 (238.15 K, selected summary of literature data, temp range 15.74–238.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C):
log (H/atm) = 8.18 – 1469.55/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)
2980 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
2478.8 (calculated-QSAR, Nirmalakhandan & Speece 1988)
3058 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
1.08 (shake flask, Log P Database, Hansch & Leo 1987)
1.08 (recommended, Sangster 1993)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k_{OH}* = (4.75 ± 0.48) × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 297–434 K, with estimated lifetime of ~1.5 yr (flash photolysis-resonance fluorescence, Atkinson et al. 1975)
k_{OH} = (3.4 ± 0.7) × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow-LMR, Howard & Evenson 1976a)
k_{OH}* = (4.25 ± 0.28) × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 253–427 K, with calculated lifetime of 16–25 yr in troposphere (discharge flow-resonance fluorescence, Chang & Kaufman 1977)
k_{OH} = 4.8 × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} at 298 K with lifetime of 43 yr in troposphere, measured range 250–350 K (FP-RF, Watson et al. 1977; quoted, Altshuller 1980)
k_{OH} = (2.76 ± 0.35) × 10^9 cm^3 $molecule^{-1}$ s^{-1} at 297 K (relative rate, Paraskevopoulos et al. 1981)
k_{OH}(calc) = 6.8 × 10^{-15} cm^3 $molecule^{-1}$ s^{-1}, and k_{OH}(obs.) = 4.68 × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR [structure-activity relationship], Atkinson 1985)
k_{OH}* = 4.68 × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
k_{OH} = 4.7 × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} with an estimated tropospheric lifetime of 4.3 yr, Bunce et al. 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: disappearance $t_{½}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); lifetime of 44 yr in troposphere (Altshuller 1980);
estimated tropospheric lifetime of 4.3 yr as global average for the reaction with hydroxyl radical in air (Bunce et al. 1991);
estimated tropospheric lifetime of 7.5 yr and 15.8 yr by rigorous calculation (Nimitz & Skaggs 1992).

TABLE 5.1.4.4.1
Reported aqueous solubilities and vapor pressures of chlorodifluoromethane (HCFC-22) at various temperatures

$$S/(\text{wt\%}) = 0.8171 - 3.5818 \times 10^{-2} \cdot (t/°C) + 8.0081 \times 10^{-4} \cdot (t/°C)^2 - 1.0075 \times 10^{-5} \cdot (t/°C)^3 + 6.9823 \times 10^{-8} \cdot (t/°C)^4 \quad (1)$$

Aqueous solubility		Vapor pressure	
Horvath 1982		Stull 1947	
summary of literature data		summary of literature data	
t/°C	S/g·m⁻³	t/°C	P/Pa
10	5296	–122.8	133.3
20	3510	–110.2	666.6
25	2899	–103.7	1333
30	2428	–96.5	2666
40	1783	–88.6	5333
50	1402	–83.4	7999
60	1180	–76.4	13332
70	1052	–65.8	26664
80	972.8	–53.6	53329
		–40.8	101325
eq. 1	S/(wt%)		
		mp/°C	–160.0

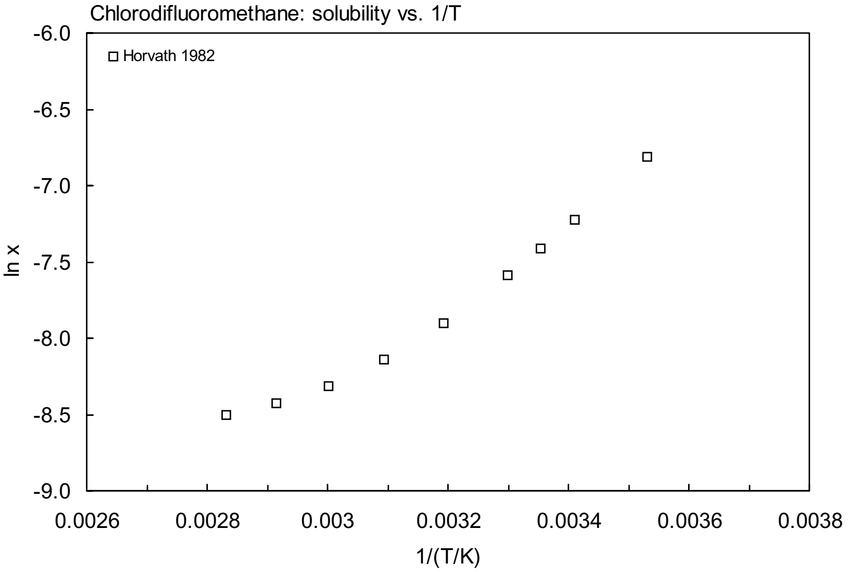
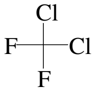


FIGURE 5.1.4.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for chlorodifluoromethane.

5.1.4.5 Dichlorodifluoromethane (CFC-12)



Common Name: Dichlorodifluoromethane
Synonym: difluorodichloromethane, Freon 12, CFC-12
Chemical Name: dichlorodifluoromethane
CAS Registry No: 75-71-8
Molecular Formula: CF_2Cl_2
Molecular Weight: 120.914
Melting Point (°C):
 –158.0 (Weast 1982–83; Dean 1985; Lide 2003)
Boiling Point (°C):
 –29.8 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 20°C):
 1.3110 (25°C, Kirk-Othmer 1985)
 1.3292, 1.3113 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
 92.2 (Stephenson & Malanowski 1987)
 81.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 20.112 (bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 4.14 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:

Water Solubility (g/m^3 or mg/L at 25°C):
 280 (DuPont 1966; quoted, Horvath 1982; Riddick et al. 1986)
 276 (Gmelins 1974)
 280 (shake flask-GC, Pearson & McConnell 1975)
 300 (recommended, Horvath 1982)
 280 (Verschueren 1983; Dean 1985; Kirk-Othmer 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
 745000, 1031000 (20°C, 30°C, static method, Gilkey et al. 1931)
 101325 (–29.8°C, summary of literature data, temp range –118.5 to –29.8°C, Stull 1947)
 214220 (calculated-Antoine eq., Weast 1975)
 log (P/mmHg) = 6.82101 – 839.622/(t/°C + 242.861); temp range –101 to + 6°C (Antoine eq., Kudchadker et al. 1979)
 566500, 769940 (20°C, 30°C, Verschueren 1983)
 566600 (20°C, quoted, Riddick et al. 1986)
 log (P/kPa) = 5.94591 – 839.622/(242.861 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
 651040 (interpolated-Antoine eq.-IV, Stephenson & Malanowski 1987)
 log (P_L/kPa) = 5.94677 – 839.6/(–30.311 + T/K); temp range 173–244 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 log (P_L/kPa) = 6.0058 – 860.828/(–28.11 + T/K); temp range 173–240 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 log (P_L/kPa) = 5.92289 – 826.707/(–32.274 + T/K); temp range 236–285 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 log (P_L/kPa) = 6.30541 – 1035.857/(–1.496 + T/K); temp range 282–345 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 7.51271 - 2016.711/(132.578 + T/K)$; temp range 341–385 K (Antoine eq.-V, Stephenson & Malanowski 1987)
$\log (P/mmHg) = 52.5701 - 2.2537 \times 10^3/(T/K) - 18.265 \cdot \log (T/K) + 1.298 \times 10^{-2} \cdot (T/K) + 2.0286 \times 10^{-13} \cdot (T/K)^2$; temp range 115–385 K (vapor pressure eq., Yaws 1994)
123390 (248.15 K, selected and summary of literature data, temp range 115.16–249.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
151960 (calculated-P/C, Mackay & Wolkoff 1973; quoted, Roberts & Dändliker 1983)
43080 (calculated-$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
22800 (estimated, Roberts 1984)
28704 (19.93°C, equilibrium cell-GC, measured range 0–40°C, Warner & Weiss 1985)
$\log K_{AW} = 5.811 - 1399/(T/K)$; temp range: 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)
304000 (20–25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)
39557 (computed value, Yaws et al. 1991)
26566 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
26810 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
$\log K_{AW} = 5.739 - 1380/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log $K_{OW:}$
2.16 (shake flask-GC, Hansch et al. 1975)
2.21 (calculated-fragment const., Rekker & de Kort 1979)
2.16 (recommended, Sangster 1993)
2.16 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
2.05 (soil, selected, Jury et al. 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization: half-life of about few minutes (Mills et al. 1982); loss half-lives in marine mesocosm were estimated to be 20 d in spring at 8–16°C and $t_{½}$ = 13 d in winter at 3–7°C (Wakeham et al. 1983).
Photolysis: photolytic dissociation of atmospheric $CFCl_3$ and CF_2Cl_2 gives chlorine atoms which destroys the ozone layer, these halomethanes may remain at altitudes of 20–40 km for 40–150 yr and will reach saturation values of 10–30 times the present levels (Molina & Rowland 1974).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}* < 0.1 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 297.3 K, measured range 297–423.8 K (flash photolysis-RF, Atkinson et al. 1975)
$k_{OH} < 0.4 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 296 K (discharge flow-LMR, Howard & Evenson 1976a)
$k_{OH} < 0.012 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 298 K (relative rate method, Cox et al. 1976)
photooxidation $t_{½}$ = 2118–21180 h in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991)
$k_{OH} < 4 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (Atkinson 1985)
$k_{OH} < 4 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} with estimated tropospheric lifetime of > 50 yr for a global average concentration of OH radical (Bunce et al. 1991).
$k_{OH} < 1 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)
Hydrolysis:
Biodegradation: aqueous aerobic $t_{½}$ = 672–4320 h, based on acclimated aerobic screening test data for trichlorofluoromethane (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 2688–16128 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} > 10$ d from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
residence time of about 50 yr in N. troposphere, estimated by one-compartment nonsteady state model (Singh et al. 1978) and
residence time of 60–70 yr by two-compartment nonsteady state model (Singh et al. 1979);
estimated residence time in troposphere about 1 year (Lyman 1982);
$t_{1/2}$ = 2118–21180 h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);
estimated global average tropospheric lifetime $\tau > 50$ yr for the reaction with hydroxyl radical in air (Bunce et al. 1991).

Surface water: $t_{1/2}$ = 672–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

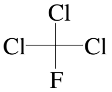
Ground water: $t_{1/2}$ = 1344–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated $t_{1/2}$ ~10000 d for volatilization loss from soil (Jury et al. 1990);
$t_{1/2}$ = 672–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

5.1.4.6 Trichlorofluoromethane (CFC-11)



Common Name: Trichlorofluoromethane
Synonym: Arcton 11, fluorotrichloromethane, fluorocarbon-11, Freon-11, Frigen 11, R 11, CFC-11
Chemical Name: trichlorofluoromethane, fluorotrichloromethane
CAS Registry No: 75-69-4
Molecular Formula: $CFCl_3$
Molecular Weight: 137.368
Melting Point (°C):
 –110.44 (Lide 2003)
Boiling Point (°C):
 23.7 (Lide 2003)
Density (g/cm^3 at 20°C):
 1.4879, 1.4760 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
 93.1 (Stephenson & Malanowski 1987)
 97.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 25.02, 25.06 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 6.895 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
 1400 (21°C, Irmann 1965; Chiou & Freed 1977)
 1100 (20°C, DuPont 1966; quoted, Riddick et al. 1986)
 1100 (20°C, Pearson & McConnell 1975)
 1100 (Verschueren 1977,1983)
 1080 (recommended, Horvath 1982)
 1080 (30°C, Horvath 1982)
 1400 (Dean 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 88550* (19.895°C, measured range –36.673 to 19.895°C, Osborne et al. 1941)
 log (P/mmHg) = 18.54101 – 1841.72/(T/K) – 3.8423.log (T/K); temp range 236.487–296.822 K (static method-manometry, Osborne et al. 1941)
 101325* (23.7°C, summary of literature data, temp range –84.3 to 23.7°C, Stull 1947)
 95670 (calculated-Antoine eq., Weast 1972–73)
 log (P/mmHg) = [–0.2185 × 6424.1/(T/K)] + 7.563786; temp range –84.3 to 13.1°C (Antoine eq., Weast 1972–73)
 88500 (20°C, Pearson & McConnell 1975)
 106390 (Antoine eq., Reid et al. 1977)
 106349 (20°C, calculated-Antoine eq., Kudchadker et al. 1979)
 log (P/mmHg) = 6.89396 – 1074.04/(t/°C + 237.276); temp range –37 to 20°C (Antoine eq., Kudchadker et al. 1979)
 91580 (20°C, Verschueren 1983)
 log (P/kPa) = 6.01333 – 1044.954/(237.102 + t/°C); temp range –36.67 to 19.89°C (Antoine eq. derived from exptl data of Osborne et al. 1941, Boublik et al. 1984)
 107010 (Daubert & Danner 1985)

102200 (selected, Riddick et al. 1986)

log (P/kPa) = 6.01886 – 1047.04/(237.276 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

106340 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.99210 – 1032.23/(–37.85 + T/K); temp range 213–249 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.99652 – 1034.048/(–37.672 + T/K); temp range 213–301 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.03083 – 1053.874/(–34.955 + T/K); temp range 295–363 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.36472 – 1285.088/(–0.653 + T/K); temp range 357–429 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.75501 – 2744.806/(196.225 + T/K); temp range 424–486 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P/mmHg) = 44.0884 – 2.5022 × 10^3/(T/K) –14.193·log (T/K) + 7.8086 × 10^{-3}·(T/K) + 1.3769 × 10^{-13}·$(T/K)^2$; temp range 162–471 K (vapor pressure eq., Yaws 1994)

10640 (selected summary of literature data, temp range 162.05–313.15 K, Xiang 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

81200 (20°C, Pearson & McConnell 1975)

11650 (calculated-P/C, Neely 1976)

11050 (20°C, calculated-P/C, Mackay & Shiu 1981)

11044 (20°C, calculated-P/C, Mabey et al. 1982)

11754 (estimated-P/C, Lyman 1985)

ln K_{AW} = 9.25 – 2372/(T/K); measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)

ln K_{AW} = 10.50 – 2652/(T/K); measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith 1983)

7925 (19.93°C, equilibrium cell-GC, measured range 0–40°C, Warner & Weiss 1985)

9827 (interpolated data of Warner & Weiss 1985; Howard 1990)

5907 (gas stripping-GC, Warner et al. 1987)

10234* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm·m^3/mol)] = 9.480 – 3513/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

11144 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

12341 (computed value, Yaws et al. 1991)

8019 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

7824 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

log K_{AW} = 5.023 – 1324/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

2.53 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)

2.53 (recommended, Sangster 1993)

2.53 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.92 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

1.95 (calculated, Klöpffer et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

2.20 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

2.31, 2.42, 2.16, 2.21 (estimated-K_{OW}, Karickhoff 1985)

2.13, 2.26 (estimated-S, Karickhoff 1985)

2.20 (best estimate, Karickhoff 1985)

2.13 (average from estimates of K_{OW} and S, Karickhoff 1985; quoted, Neely & Blau 1985)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2}$ = 3.4 h from Henry's law constant for a river 1.0 m deep with a 3 m/s wind and 1 m/s current (Lyman et al. 1982; Cadena et al. 1984; quoted, Howard 1990);

$t_{1/2}$ ~ few minutes (Mills et al. 1982).

Photolysis: photolytic dissociation of atmospheric $CFCl_3$ and CF_2Cl_2 gives chlorine atoms which destroys the ozone layer, these halomethanes may remain at altitudes of 20–40 km for 40–150 yr and will reach saturation values of 10–30 times the present levels (Molina & Rowland 1974).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}* < 0.1 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 296.8 K, measured range 297–424 K (flash photolysis-resonance fluorescence, Atkinson et al. 1975)

k_{OH} < 0.05 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (discharge flow-LMR, Howard & Evenson 1976a)

k_{OH} < 0.005 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 298 K (relative rate method, Cox et al. 1976)

k_{OH} < 1.0 × 10^{-17} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

Hydrolysis: estimated exptl. rate constant k = 9.5 × 10^{-7} d^{-1}, based on carbon tetrachloride (Neely 1985).

Biodegradation: aqueous aerobic $t_{1/2}$ = 4032–8640 h, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 16128–34560 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ > 10 d from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976);

estimated residence time about 1000 yr in troposphere for the reaction with OH radical (CEQ 1975);

estimated residence time in N. troposphere about 15–20 yr by one-compartment nonsteady state model and 40–45 yr in troposphere by two-compartment nonsteady state model (Singh et al. 1979);

estimated residence time in troposphere about 1–6 yr (Lyman 1982);

$t_{1/2}$ = 14.7–147 yr, based on an measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 4032–8640 h, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2}$ = 8640–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.4.6.1
Reported vapor pressures and Henry's law constants of trichlorofluoromethane (CFC-11) at various temperatures and the coefficients for the vapor pressure equations

Vapor pressure				Henry's law constant	
Osborne et al. 1941		Stull 1947		Ashworth et al. 1988	
static method		summary of literature data		EPICS-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m^3/mol)
–36.673	6313	–84.3	133.3	10	5431
–21.825	14416	–67.6	666.6	15	6890
–6.887	29811	–59.0	1333	20	8147
–2.352	44611	–49.7	2666	25	10234
–10.362	61790	–39.0	5333	30	12362
15.108	74147	–32.3	7999		
19.895	88550	–23.0	13332	ln [H/(atm·m^3/mol)] = A – B/(T/K)	
23.662	101325	–9.10	26664	A	9.480
		6.80	53329	B	3513
		23.7	101325		
		mp/°C	-		

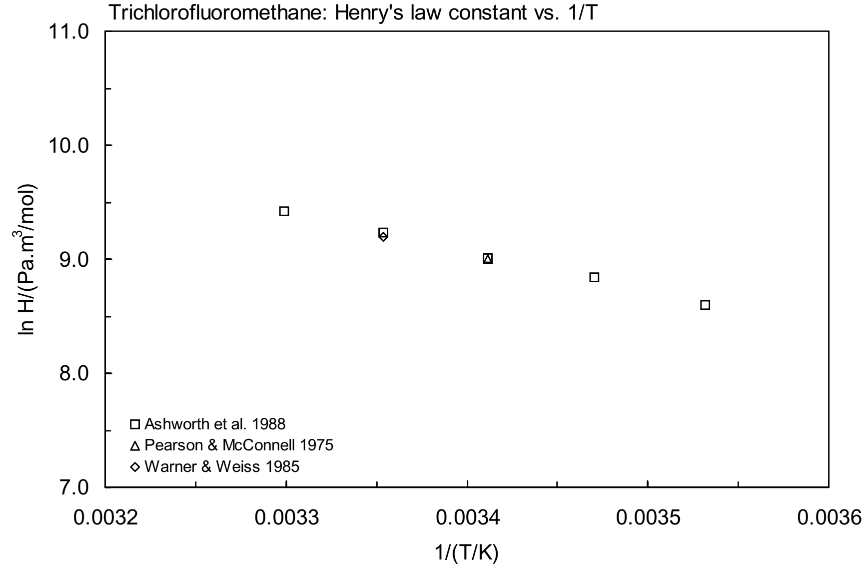
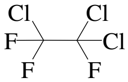


FIGURE 5.1.4.6.1 Logarithm of Henry's law constant versus reciprocal temperature for trichlorofluoromethane.

5.1.4.7 1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)



Common Name: 1,1,2-Trichloro-1,2,2-trifluoroethane
Synonym: CFC-113, Freon 113, 1,2,2-trifluoro-1,1,2-trichloroethane
Chemical Name: 1,1,2-trichloro-1,2,2-trifluoroethane, Arklone
CAS Registry No: 76-13-1
Molecular Formula: $C_2Cl_3F_3$, $CClF_2CCl_2F$
Molecular Weight: 187.375
Melting Point (°C):

–36.22	(Lide 2003)

Boiling Point (°C):

47.7	(Lide 2003)

Density (g/cm^3 at 20°C):

1.5635	(25°C, Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

119.8	(20°C, calculated-density)
129.5	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):

170	(DuPont 1966; quoted, Riddick et al. 1986)
170	(shake flask-GC, Rauws et al. 1973)
170	(20°C, Jones et al. 1977/1978)
166.4*	(summary of literature data, Horvath 1982)
170	(Dean 1985)
170	(recommended, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

53329*	(30.2°C, summary of literature data, temp range –68.0 to 47.4°C, Stull 1947)
48476*	(static method-isoteniscope, measured range 273.35–318.10 K, Hiraoka & Hildebrand 1963)
39040	(calculated-Antoine eq., Weast 1972–73)
48320	(calculated-Antoine eq., Boublik et al. 1984)
48480	(selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.6783 - 1499.2/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/\text{kPa}) = 5.91657 - 1094.37/(-39.61 + T/K)$; temp range 273–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.01641. - 1115.812/(-42.515 + T/K)$; temp range 238–364 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.53093 - 1500.489/(12.469 + T/K)$; temp range 360–473 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.95163 - 1082.588/(-46.427 + T/K)$; temp range 297–317 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 33.7911 - 2.5323 \times 10^3/(T/K) - 9.3175 \cdot \log(T/K) + 1.455 \times 10^{-8} \cdot (T/K) + 2.914 \times 10^{-6} \cdot (T/K)^2$; temp range 238–481 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

32320*	(EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm m^3/mol)] = 9.649 – 3243/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

53300	(calculated-P/C, Howard 1990)
49132	(computed value, Yaws et al. 1991)
24616	(20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

log K_{AW} = 5.375 – 1281/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

3.16	(HPLC-k′ correlation, McDuffie 1981; quoted, Howard 1990, Sangster 1993))
3.16	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.531, 1.041	(calculated-S, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

2.28, 2.41	(soil, calculated-K_{OW}, calculated-S, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2}$ = 4 h was estimated for a model river 1 m deep flowing 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: both aqueous and atmospheric photolysis half-lives are infinite (Howard et al. 1991).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} < 0.3 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow-laser magnetic resonance, Howard & Enenson 1976b)

photooxidation $t_{1/2}$ = 40–1000 yr in troposphere, based on measured rates with singlet oxygen (Davidson et al. 1978; Pitts Jr. et al. 1974; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2}$ = 4320–8640 h, based on a relative resistance of completely halogenated aliphatics to biodegrade; aqueous anaerobic $t_{1/2}$ = 17280–34560 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

degradation rates in microcosms at 20°C: k = 7.6×10^{-3} d^{-1} by control buffer with $t_{1/2}$ = 90 d, k = 9.1×10^{-3} d^{-1} by redox buffer with $t_{1/2}$ = 75 d, k = 1.2×10^{-2} d^{-1} by 1 mg/L redox-hematin with $t_{1/2}$ = 57 d, k = 1.6×10^{-2} d^{-1} by 2 mg/L redox-hematin with $t_{1/2}$ = 43 d, k = 9.9×10^{-2} d^{-1} by purged leachate with $t_{1/2}$ = 7 d, and k = 0.14 d^{-1} by leachate with $t_{1/2}$ = 5 d (Lesage et al. 1992).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ > 10 d from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2}$ = 40–1000 yr in troposphere, based on measured rates with singlet oxygen (Davidson et al. 1978; Pitts Jr. et al. 1974; quoted, Howard et al. 1991);

$t_{1/2}$ = 20 yr in troposphere (Dilling 1982; quoted, Howard 1990).

Surface water: $t_{1/2}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2}$ = 1440–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.4.7.1

Reported aqueous solubilities, vapor pressures and Henry's law constants of 1,1,2-trichloro-1,2,2-trifluoroethane (CFC-113) at various temperatures

$$S/(\text{wt}\%) = 1.0648 \times 10^{-2} + 3.51135 \times 10^{-4}\cdot(t/°C) - 6.1331 \times 10^{-6}\cdot(t/°C)^2 + 6.70235 \times 10^{-8}\cdot(t/°C)^3 \quad (1)$$

$$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K) \quad (2)$$

Aqueous solubility		Vapor pressure				Henry's law constant	
Horvath 1982		Stull 1947		Hiraoka & Hildebrand 1963		Ashworth et al. 1988	
summary of literature data		summary of literature data		static method isoteniscope		EPICS-GC	
t/°C	$S/g\cdot m^{-3}$	t/°C	P/Pa	t/°C	P/Pa	t/°C	$H/(Pa\ m^3/mol)$
0	106.5	–68.0	133.3	0.20	17252	10	15604
10	136.1	–49.4	666.6	5.0	21278	15	21785
20	157.5	–40.3	1333	10.3	26731	20	24825
25	166.4	–30.0	2666	10.45	26891	25	32323
30	174.7	–18.5	5333	15.1	32597	30	32525
40	191.7	–11.2	7999	20.0	39970		
50	212.5	–1.70	13332	25.05	48476	eq. 2	$H/(atm\ m^3/mol)$
60	241.1	13.5	26664	30.1	58528	A	9.649
70	281.6	30.2	53329	35.1	69887	B	3243
80	338.0	47.4	101325	40.1	82286		
				44.95	96898		
eq.1	S/wt%	mp/°C	–35				

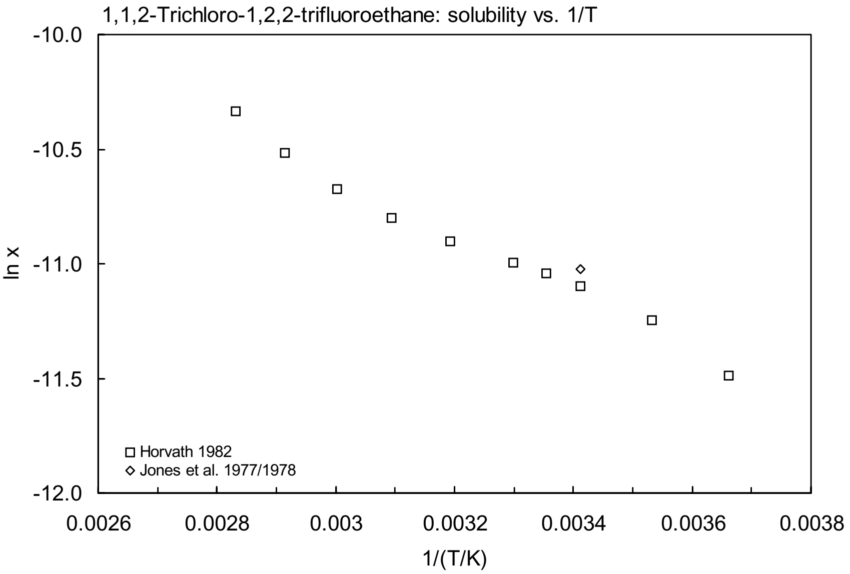


FIGURE 5.1.4.7.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

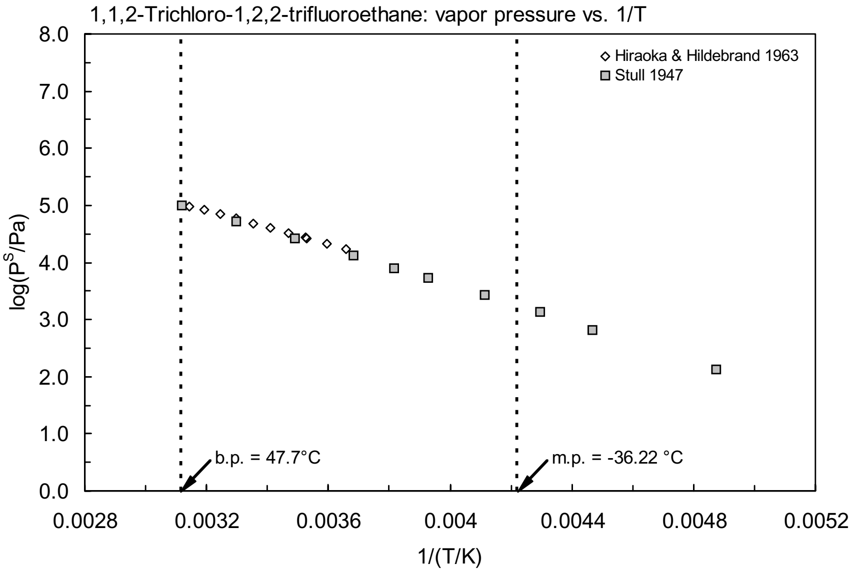


FIGURE 5.1.4.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

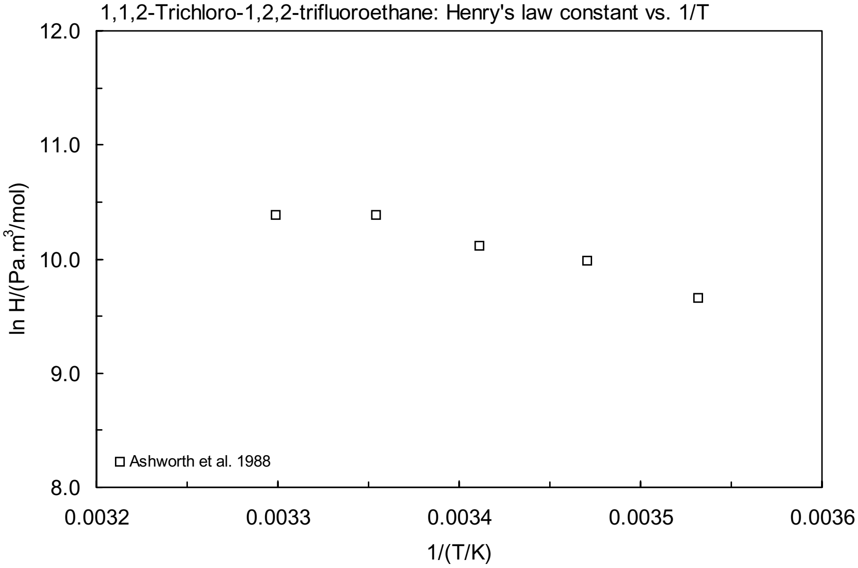
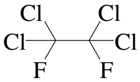


FIGURE 5.1.4.7.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

5.1.4.8 1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112)



Common Name: 1,1,2,2-Tetrachloro-1,2-difluoroethane
Synonym: Freon-112, CFC-112
Chemical Name: 1,2-difluorotetrachloroethane
CAS Registry No: 76-12-0
Molecular Formula: $C_2F_2Cl_4$, $Cl_2FCCFCl_2$
Molecular Weight: 203.830
Melting Point (°C):
26.55 (Riddick et al. 1986)
24.9 (Lide 2003)
Boiling Point (°C):
92.80 (Riddick et al. 1986; Lide 2003)
Density (g/cm³ at 20°C):
1.6447 (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
145.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of vaporization, ΔH_V (kJ/mol):
35 (Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
3.666 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
120 (DuPont 1966; quoted, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6106 (20°C, measured range 10–91.5°C, Hovorka & Geiger 1933)
7609 (calculated-Antoine eq., Boublik et al. 1984)
$\log(P/kPa) = 9.94341 - 4259.092/(444.991 + t/°C)$, temp range 10–91.5°C (Antoine eq. derived from.exptl. data of Hovorka & Geiger 1933, Boublik et al. 1984)
8770 (selected, Riddick et al. 1986)
$\log(P/kPa) = 7.2972 - 1929.27/(T/K)$; temp range not specified (Antoine eq., Riddick et al. 1986)
$\log(P_S/kPa) = 6.50788 - 1526.24/(-28.93 + T/K)$; temp range 235–293 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log(P_L/kPa) = 6.67780 - 1567.8/(-29.58 + T/K)$; temp range 301–365 K (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log(P_L/kPa) = 5.97313 - 1239.993/(-53.468 + T/K)$; temp range 312–362 K (Antoine eq., Stephenson & Malanowski 1987)
$\log(P/mmHg) = -38.1282 - 1.2604 \times 10^3/(T/K) + 23.347 \cdot \log(T/K) - 3.4436 \times 10^{-2} \cdot (T/K) + 1.7407 \times 10^{-5} \cdot (T/K)^2$; temp range 299–551 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
9869 (calculated-$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
248, 1426 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
161419 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
2.82 (shake flask, Log P Database, Hansch & Leo 1987)
3.73 (Howard 1990)
2.82 (recommended, Sangster 1993)

Bioconcentration Factor, log BCF:

1.62	(estimated-S, Lyman et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

2.50	(soil, estimated-linear regression with S, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization: volatilization $t_{½}$ ~ 4.0 h from a model river 1 m deep flowing 1 m/s with a wind velocity of 3 m/s, based on estimated Henry's law constant (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Photolysis: will not undergo direct photolysis in the troposphere (quoted, Howard 1990).

Oxidation: inert to react with photochemically produced radicals and ozone molecules (Dilling 1982; Atkinson 1985,1987; quoted, Howard 1990).

Hydrolysis: not an environmentally significant fate process (DuPont 1980; quoted, Howard 1990).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: by analogy to other Freon compounds, Freon-112 is predicted to have a stratospheric lifetime on the order of several decades (Chou et al. 1978; quoted, Howard 1990).

Surface water: will volatilize very rapidly (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Ground water: will volatilize very rapidly (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Sediment: will volatilize very rapidly from soil surfaces (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Soil:

Biota:

5.1.5 FLUOROALKANES AND FLUOROALKENES

A large number of stable and volatile fluorinated and chlorinated alkanes and alkenes have been synthesized and used, primarily as refrigerants. These "freons" have been implicated as the cause of observed reductions in stratospheric ozone levels, thus permitting greater penetration of ultraviolet radiation to the Earth's surface. Their high vapor pressures and relatively low solubilities in water result in high Henry's law constants or air-water partition coefficients. Fate calculations show that when released into the environment virtually the total mass of these substances will partition to the atmospheric compartment. Levels in water, soil, sediments and biota are likely to be very low and of little concern. Accordingly, there is little merit in compiling detailed data on these substances in a format comparable to that, for example, the chlorobenzenes or PCBs.

In the interest of conserving space in this handbook, a compact tabular presentation format has been adopted. Table 5.1.5.1 lists the chemical name, and its freon number (if applicable), molecular formula, molar weight and melting and boiling points. These data are available for virtually all substances in this group. Also shown in this table is the availability, expressed as a tick mark, of data on vapor pressure, solubility in water, octanol-water partition coefficient (K_{OW}) and the second order reaction rate constant with hydroxyl radicals. This rate constant is the critical determinant of persistence in the atmosphere. Tables 5.1.5.2 to Table 5.1.5.5 list the compounds and give the available property data with citations.

TABLE 5.1.5.1
Summary of physical constants for fluoroalkanes and fluoroalkenes

Compound	Freon no.	CAS no.	Molecular formula	Molecular weight g/mol	mp°C	bp°C	LeBas molar volume, V_M cm³/mol	Properties** S	P	K_{OW}	k_{OH}
Fluoroalkanes											
Fluoromethane	HFC-41	593-53-3	CH_3F	34.05	–141.8	–79.1	34.6	✓	✓	✓	✓
Difluoromethane	HFC-32	75-10-5	CH_2F_2	52.02	–136	–51.6	39.6	✓	✓	✓	✓
Trifluoromethane	HFC-23	75-46-7	CHF_3	70.01	–155.2	–82.16	44.6	✓	✓	✓	✓
Tetrafluoromethane	FC-14	75-73-0	CF_4	88.005	–183.60	–128.0	49.6	✓	✓	✓	✓
Chlorofluoromethane	HCFC-31	593-70-4	CH_2ClF	68.48	–133	–9.1	55.5	✓	✓		✓
Dichlorofluoromethane	HCFC-21	75-43-4	$CHCl_2F$	102.92	–135	8.92	76.4	✓	✓	✓	✓
Chlorodifluoromethane	HCFC-22*	75-45-6	$CHClF_2$	86.47	–160	–40.7	60.5	✓	✓	✓	✓
Chlorotrifluoromethane	CFC-13	75-72-9	CF_3Cl	104.46	–181	–82	65.5	✓	✓	✓	✓
Dichlorodifluoromethane	CFC-12*	75-71-8	CCl_2F_2	120.91	–155	–29.8	81.4	✓	✓	✓	✓
Trichlorofluoromethane	CFC-11*	75-69-4	$CFCl_3$	137.37	–111	23.82	97.3	✓	✓	✓	✓
Fluoroethane	HFC-161	353-36-6	CH_3CH_2F	48.06	–143	–37.7	56.8	✓	✓		✓
1,1-Difluoroethane	HFC-152a	75-37-6	CH_3CHF_2	66.05	–117	–24.7	61.8	✓	✓	✓	✓
1,2-Difluoroethane	HFC-152	624-72-6	CH_2FCH_2F	66.05		26	61.8	✓			✓
1,1,1-Trifluoroethane	HFC-143a	420-46-2	CF_3CH_3	84.04	–111.3	–47.4	66.8	✓	✓		✓
1,1,2-Trifluoroethane	HFC-143b	430-66-0	CH_2FCHF_2	84.04	–84	3.7	66.8	✓			✓
1,1,2,2-Tetrafluoroethane	HFC-134	359-35-3	CHF_2CHF_2	102.03	–89	–19.9	71.8	✓	✓		✓
1,1,1,2-Tetrafluoroethane	HFC-134a	811-97-2	CH_2FCF_3	102.03	–103.3	–26.08	71.8	✓	✓	✓	✓
Pentafluoroethane	HFC-125	354-33-6	CF_3CHF_2	120.02	–103	–48.5	76.8	✓	✓		✓
Hexafluoroethane	FC-116	76-16-4	CF_3CF_3	138.01	–100.6	–79	81.8	✓	✓	✓	
1-Chloro-2-fluoroethane	HCFC-151	762-50-5	CH_2FCH_2Cl	82.5	<–50	52.8	77.7	✓			
1-Chloro-1,1-difluoroethane	HCFC 142b	75-68-3	CH_3CClF_2	100.5	–130.8	–9.5	82.7	✓	✓	✓	✓
1-Chloro-1,1,2-trifluoroethane	HCFC-133a	421-04-5	CH_2ClCF_3	118.49		12	87.7				✓
1-Chloro-1,2,2,2-tetrafluoroethane	HCFC-124	2837-89-0	$CHClFCF_3$	136.5		–11.0	92.7	✓	✓	✓	✓
1-Chloropentafluoroethane	CFC-115	76-15-3	$CClF_2CF_3$	154.47	–99.4	–39.1	97.7	✓	✓	✓	
1,1-Dichloro-1-fluoroethane	HCFC-141b	1717-00-6	CCl_2FCH_3	116.95	–103.5	32.0	98.6	✓	✓	✓	✓
1,2-Dichloro-1,1-difluoroethane	HCFC-132b	1649-08-7	$CClF_2CH_2Cl$	134.97	–101.2	46.8	103.6				✓
1,1-Dichlorotrifluoroethane	HCFC-123	306-83-2	$CHCl_2CF_3$	152.93	–107	27.6	108.6	✓	✓		✓
1,2-Dichloro-1,1,2,2-tetrafluoroethane	CFC-114	76-14-2	$CClF_2CClF_2$	170.92	–93.9	3.8	113.6	✓	✓	✓	
1,1-Dichloro-1,2,2,2-tetrafluoroethane	CFC-114a	374-07-2	CCl_2FCF_3	170.92	–56.6	3.4	113.6	✓		✓	
1,1,1-Trichloro-2,2,2-trifluoroethane	CFC-113a	354-58-5	CCl_3CF_3	187.38	14.2	47.57	129.5		✓		
1,1,2-Trichloro-1,2,2-trifluoroethane	CFC-113*	76-13-1	CCl_2FCClF_2	187.38	–36.4	47.7	129.5	✓	✓	✓	

1,1-Difluorotetrachloroethane			$CClF_2CCl_3$	203.83	38	91	145.4			✓	
1,1,2,2-tetrachloro-1,2-difluoroethane	CFC-112*	76-12-0	CCl_2FCCl_2F	203.83	25	93	145.4	✓	✓	✓	
2-Fluoropropane	HFC-281ea	420-26-8	CH_3CHFCH_3	62.09	–133.4	–10	79.0	✓	✓		
1,1,2,2,3-Pentafluoropropane	HFC-245ca	679-86-7	$CH_2FCF_2CHF_2$	134.05			99.0		✓		✓
1,1,1,3,3-Pentafluoropropane	HFC-245fa	460-73-1	$CF_3CH_2CHF_2$	134.05			99.0		✓		
1,1,1,2,2-Pentafluoropropane	HFC-245cb	1814-88-6	$C_3H_3F_5$	134.05		–17.4	99.0		✓		✓
1,1,1,2,3,3-Hexafluoropropane	HFC-236ea	431-63-0	CHF_2CHFCF_3	152.04		6.1	104.0		✓		✓
1,1,1,3,3,3-Hexafluoropropane	HFC-236fa	690-39-1	$CF_3CH_2CF_3$	152.04	–93.6	–1.0	104.0		✓		✓
1,1,1,2,3,3,3-Heptafluoropropane	HFC-227ea	431-89-0	CF_3CHFCF_3	170.03	–131	–16.4	109.0		✓		✓
Octafluoropropane	FC-218	76-19-7	$CF_3CF_2CF_3$	188.02	–183	–38	114.0	✓	✓		
Trichlorotrifluoropropane									✓		
1-Chloro-2,2,2-trifluoropropane			$CH_2ClCH_2CF_3$	132.51	–106.2	45.1	109.9	✓	✓		
Perfluorobutane	FC-3110	355-25-9	C_4F_{10}	238.03	–129.1	–1.9	146.2		✓		
Perfluorocyclobutane	FC-118	115-25-3	C_4F_8	200.03	–40.19	–5.9	120.3	✓	✓		
Perfluoropentane	FC-87	678-26-2	C_5F_{12}	288	–10	29.2	178.4		✓		
Perfluorocyclopentane		376-77-2							✓		
Perfluoro-2-methylcyclopentane									✓		
Perfluoro-3-methylcyclopentane									✓		
Perfluorocyclohexane		355-68-0	C_6F_{12}	300.05	48	52	178.2		✓		
Perfluorohexane	FC-72	355-42-0	C_6F_{14}	338.04	–88.2	56.6	210.6		✓		
Fluoroalkenes											
Fluoroethene	HFC-1141	75-02-5	$CHF{=}CH_2$	46.05	–160	–72.2	49.4	✓			
1,1-Difluoroethene	HFC-1132a	75-38-7	$CF_2{=}CH_2$	64.04	–144	-82	54.4	✓		✓	
Tetrafluoroethene	FC-1114	116-14-3	$CF_2{=}CF_2$	100.02	–131.15	–75.9	64.4	✓	✓		
Chlorotrifluoroethene	CFC-1113	79-38-9	$CClF{=}CF_2$	116.47	–158.2	–26.2	80.3		✓		
1,2-Dichloro-1,2-difluoroethene	CFC-1112	311-81-9	$CClF{=}CClF$	132.92	–119.6	21.1	96.2		✓		
1,1-Dichloro-2,2-difluoroethene	CFC-1112a	79-35-6	$CCl_2{=}CF_2$	132.925	–115	19	96.2		✓		
3-Fluoropropene		818-92-8	$CH_2FCH{=}CH_2$	60.07		–3.0	71.6	✓			
Hexafluoropropene	FC-1216	116-15-4	C_3F_6	150.002	–156.5	–29.6		✓	✓		

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* See Section 5.1.4. Mixed halogenated hydrocarbons.

** S = water solubility; P = vapor pressure; K_{OW} = octanol-water partition coefficient; k_{OH} = second order reaction rate constant with hydroxyl radicals.

TABLE 5.1.5.2
Aqueous solubilities for fluoroalkanes and fluoroalkenes

Compound	Temp.°C	Solubility	Unit	Range, wt %	Mole fraction *x*	Temp./pressure range	Reference
Fluoroalkanes							
Fluoromethane	25	0.2001	wt %	0.4227–0.08005	0.001061	0–80°C, 1 atm partial pressure	1
	25	2390	ppm (wt)				2
Difluoromethane	25	4390	ppm (wt)				2
Trifluoromethane	25 at 1 atm	0.09	g/100 mL	0.09–0.02		25–75°C, pressure 1–20.41 atm	1
	25	0.4087	wt %		0.001056	1 atm partial pressure	1
	25	900	ppm (wt)				2
	25	0.0733	g/100 mL			from Hine & Mookerjee (1975)	3
Tetrafluoromethane	25	0.001877	wt %	0.003892–0.001300	3.84×10^{-6}	0–50°C, 1 atm partial pressure	1
	25 at 1 atm	0.00160	g/100 mL	0.00160–0.0005		25–75°C, 1–10.2 atm	1
	25	16.0	ppm (wt)				2
	25	0.4592	$10^2L_{2,1}$, Ostwald coefficient			288–303 K, 1atm partial pressure	4
Chlorofluoromethane	25	1.0522	wt %	1.6840–0.3285	0.002790	10–50°C, 1 atm partial pressure	1
	25	10500	ppm (wt)			1 atm partial pressure	2
Dichlorofluoromethane	25 at 1 atm	1.880	g/100 mL	1.88–0.418		25–75°C, 0.068–3.40 atm	1
	25	0.95	wt %			DuPont	5
	25	18800	ppm (wt)				2
Chlorodifluoromethane	25	0.2899	wt %	0.5296–0.09728	6.055×10^{-4}	10–50°C, 1 atm partial pressure	1
	25 at 1 atm	0.277	g/100 mL	0.792–0.089		5–76.7°C, 1–33.34 atm	1
	25	0.30	wt %				5
	25	27.7	ppm (wt)				2
	25 at 1 atm	0.2899	g/100 mL			from Horvath (1982)	3
Chlorotrifluoromethane	25 at 1 atm	0.009	g/100 mL	0.009–0.004		25–75°C, 1–23.81 atm	1
	25	0.009	wt %				5
	25	90	ppm (wt)				
	25	2.253	$10^2L_{2,1}$, Ostwald coefficient			288–303 K, 1 atm partial pressure	4
Dichlorodifluoromethane	25 at 1 atm	0.030	g/100 mL	0.030–0.008		25–76.7°C, 1–6.80 atm	1
	25	0.028	wt %				5
	25 at 1 atm	0.028	g/100 mL			quoted Riddick (1986)	6
	25	300	ppm (wt)				2
	25	7.110	$10^2L_{2,1}$, Ostwald coefficient			288–303 K, 1 atm partial pressure	4
Trichlorofluoromethane	30 at 1 atm	0.1080	g/100 mL	0.108–0.031		30–75°C, 1–3.4 atm	1
	25	0.11	wt %			DuPont	5
	25	1080	ppm (wt)				1

	25	0.108	g/100 mL			from Horvath (1982)	9
Fluoroethane	25	0.2158	wt %	0.4022–02158	8.10×10^{-4}	14–25°C, 1 atm partial pressure	1
	25	2160	ppm (wt)			1 atm partial pressure	
1,1-Difluoroethane	21	0.32	wt %	0.54–0.25	8.748×10^{-4}	0–27.5°C, 1 atm partial pressure	1
	25	2500	ppm (wt)			1 atm partial pressure	2
	25 at 1 atm	0.280	g/100 mL			from Horvath (1982)	3
1,2-Difluoroethane	25	0.0157	wt %	0.012–0.02660	1.342×10^{-5}	25–80°C, saturation pressure	1
1,1,2-Trifluoroethane	25	0.01664	wt %	0.01065–0.03380	1.60×10^{-5}	0–80°C, saturated pressure	1
	30	0.011	g/100 mL	0.011–0.026		30–75°C, 0.34–2.04 atm	1
1,1,1,2-Tetrafluoroethane	37	0.0550	wt %		9.71×10^{-5}	37°C, 1 atm partial pressure	1
1,1,2,2-Tetrafluoroethane	25	0.2962	wt %	0.3299–0.4199	3.187×10^{-4}	1 atm	1
Pentafluoroethane	25	0.04995	wt %	0.05411–0.07783	4.45×10^{-5}	0–80°C, saturated pressure	1
	25	58.0	ppm (wt)				2
	25	0.0039	g/100 mL			estimated from K_{OW}	6
Hexafluoroethane	22.3	0.0050	wt %		3.805×10^{-6}	22.3°C, 0.0050 atm	1
	25	7.90	ppm (wt)				2
	25.314				9.975×10^{-7}	287–328 K, 96.6–120.5 kPa	7
1-Chloro-2-fluoroethane	25	2.4390	wt %		0.005429	saturated pressure	1
1-Chloro-1,1-difluoro-	21 at 1 atm	0.140	wt %	0.214–0.140	2.512×10^{-4}	13–21°C, 1 atm partial pressure	1
1-Chloro-1,2,2,2-tetrafluoro-	25	0.0404	g/100 mL			estimated from K_{OW}	6
1-Chloropentafluoro-	25 at 1 atm	0.0058	g/100 mL	0.0058–0.0013		25–75°C, 1–6.80 atm	1
	25	0.006	wt %				5
1,1-Dichloro-1-fluoro	25	0.066	wt %				
1,1-Dichlorotrifluoroethane	25	0.0046	wt %				8
	25	0.01857	g/100 mL			estimated from K_{OW}	6
1,2-Dichloro-1,1,2,2-tetra-	25	0.0120	wt %	0.0120–0.02662	1.061×10^{-5}	25–80°C, saturated pressure	1
	25	0.1792	wt %	0.1792–0.03487	1.586×10^{-6}	25–80°C, 1 atm partial pressure	1
	30 at 1 atm	0.009	g/100 mL	0.009–0.020		30–75°C, 0.068–0.612 atm	1
	25	0.013	wt %				5
	25	137	ppm (wt)				2
	25	0.013	g/100 mL			from Riddick (1986)	9
1,1-Dichloro-1,2,2,2-tetra-	25	0.1100	wt %	0.1197–0.1848	11.82×10^{-6}	0–80°C, saturation pressure	1
	21	0.0060	g/100 mL			from Horvath (1982)	3
1,1,2-Trichloro-1,2,2-tri-	25	0.01664	wt %	0.01065–0.003380	1.60×10^{-5}	0–80°C, saturated pressure	8
	30 at 0.34 atm	0.011	g/100 mL			30–75°C, 0.34–2.04 atm	1
	25	0.017	wt %				5
	25	170	ppm (wt)				2
	25	0.017	g/100 mL			from Riddick (1986)	9

(Continued)

TABLE 5.1.5.2 *(Continued)*

Compound	Temp.°C	Solubility	Unit	Range, wt %	Mole fraction x	Temp./pressure range	Reference
1,2-Difluorotetrachloro-	25	0.012	wt %				5
	25	0.012	g/100 mL			from Riddick (1986)	9
2-Fluoropropane	15	0.3663	wt %		0.001066	1 atm partial pressure	1
	15	3660	ppm (wt)			1 atm partial pressure	2
Octafluoropropane	15	0.001495	wt %		1.432×10^{-6}	15°C, saturated pressure	1
Perfluorocyclobutane	21	0.014	wt %		1.259×10^{-5}	21°C, 1 atm partial pressure	1
	26 at 1 atm	0.005	g/100 mL			0–37.8°C, 1–2.72 atm	1
	26	50.0	ppm (wt)				2
Fluoroalkenes							
1-Fluoroethene	80 at 34 atm	0.9312	wt %		0.003664	34 atm	1
	80 at 68 atm	1.5166	wt %		0.005988	68 atm	1
1,1-Difluoroethene	25	0.01649	wt %		4.638×10^{-5}	1 atm partial pressure	1
	25	165	ppm (wt)			1 atm partial pressure	2
Tetrafluoroethene	25	0.01585	wt %	0.04062–0.008782	2.856×10^{-5}	0–70°C, 1 atm partial pressure	1
	23 at 4.4 atm	0.001	wt %	0.001–1.274	1.78×10^{-6}	23°C, total pressure 4.4–13.45 atm	1
	25	158	ppm (wt)				2
3-Fluoropropene	13	0.007167	wt %		2.149×10^{-5}	1 atm partial pressure	1
Hexafluoropropene	25	0.01691	wt %	0.04164–0.007132	2.327×10^{-5}	0–70°C, 1 atm partial pressure	1

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TABLE 5.1.5.3
Vapor pressures for fluoroalkanes and fluoroalkenes

Compound	Temp. °C or K	P^S kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
Fluoroalkanes						
Fluoromethane				–103 – –76°C	20–116	Moles and Batuecas 1919[#]
			static	–133.1 – –78.5°C	1.33–101	Grosse et al. 1940
			literature summary	–147.3 – –78.2°C	0.1333–101.325	Stull 1947
	15.28°C	3045.3	manometer	–109–15°C	13–3045	Michels and Wassenaar 1948
	298.15 K	3824.9	literature summary	131–317 K	0.43–5880	Xiang 2002
Difluoromethane	298.16 K	1689	static	191–352 K	16.36–5828	Malbrunot et al. 1968
			comparative ebulliometry	208–237 K	49–214	Weber and Goodwin 1993
	298.174 K	1690.81	Burnett apparatus/densimeter	268–348 K	690–5409	Defibaugh et al. 1994
			isochoric	320–351 K	2919–5783.6	Sato et al. 1994
			ebulliometry (metal)	236–266 K	200–650	Weber and Silva 1994
	299.985 K	1774	manometer/densimeter	220–325 K	95–3278	Widiatmo et al. 1994
	297.15 K	1645.1	Burnett apparatus	233–351 K	177–5767.9	Fu et al. 1995
	298.15 K	1689.7	literature summary	137–351 K	5.69×10^{-2} – 5780	Xiang 2002
	308.15 K	2191	VLE			Horstmann et al. 2004
Trifluoromethane			calorimetry static	145–192 K	2.72–102.51	Valentine et al. 1962
	298.15 K	4714.9	literature summary	118–299 K	5.71×10^{-2} – 4800	Xiang 2002
Tetrafluoromethane			literature summary	–184.6 – –127.7°C	0.1333–101.325	Stull 1947
			calorimetry static	115–146 K	7–106	Smith and Pace 1969
						Bonifácio et al. 2001
			literature summary	90–228 K	1.04×10^{-1}–3740	Xiang 2002
Chlorofluoromethane	298.15 K	343.82	literature summary	138–427 K	2.28×10^{-3}–5700	Xiang 2002
Dichlorofluoromethane			isoteniscopic	–29.65–174.6°C	17.31–4894	Benning and McHarness 1940
			literature summary	–91.3–8.90°C	0.1333–101.325	Stull 1947
	298.15 K	181.67	literature summary	138–452 K	2.94×10^{-4} – 5183	Xiang 2002
Chlorodifluoromethane	22.6°C	951	manometer	22.6–96.4°C	951–4912	Booth and Swinehart 1935
	25.15°C	1050.74	isoteniscopic	–61.26–92.6°C	35.12–4652.84	Benning and McHarness 1940
			literature summary	–122.8 – –40.8°C	0.1333–101.325	Stull 1947
	50°C	1955	VLE			Leu and Robinson 1992
	65°C	2710	VLE			Leu and Robinson 1992
	70°C	3003	VLE			Leu and Robinson 1992
	75°C	3843	VLE			Leu and Robinson 1992

(Continued)

TABLE 5.1.5.3 *(Continued)*

Compound	Temp. °C or K	P^S kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
	289.10 K	811.7	isochoric	245–328 K	180–2195	Giuliani et al. 1995a
	298.15 K	1044.2	literature summary	115–369 K	4.26×10^{-4}–4988	Xiang 2002
Chlorotrifluoromethane			literature summary	–149.5 – –81.2°C	0.1333–101.325	Stull 1947
	298.15 K	3578.3	literature summary	92–302 K	4.40×10^{-4}–3890	Xiang 2002
Dichlorodifluoromethane			literature summary	–118.5 – –29.8°C	0.1333–101.325	Stull 1947
	25.338°C	656		25–111°C	656–4062	Michels et al. 1966
	298.15 K	650.91	literature summary	115–385 K	2.33×10^{-4}–4100	Xiang 2002
Trichlorofluoromethane	24.02°C	102.24	isoteniscopic	–29.65–195.65°C	1.05–4273.89	Benning and McHarness 1940
	293.055 K	88.55	calorimetry static	236–293 K	6.31–88.55	Osborne et al. 1941
	23.7°C	101.325	literature summary	–84.3–23.7°C	0.1333–101.325	Stull 1947
	298.15 K	106.4	literature summary	162–471 K	6.26×10^{-3}–4408	Xiang 2002
Fluoroethane	25.65°C	932	manometer	25.65–102.16°C	932–5028	Booth and Swinehart 1935
			static	–103.6 – –37.1°C	1.33–101	Grosse et al. 1940
	295.82 K	865.9	static	228–322 K	70–1699	Vidaurri 1975
	20°C	833.3		16–78°C	738–3197	Beyerlein et al. 1998
1,1-Difluoroethane	290.76 K	22	mercury manometer	234–291 K	0.858–22	Li and Pitzer 1956
	298.15 K	596	isochoric	239–368 K	59–3334	Zhao et al. 1992
			ebulliometry	220–273 K	23–264	Silva and Weber 1993
	295.452 K	550.01	ebulliometry	281–335 K	352–1550	Defibaugh and Morrison 1996
	298.15 K	597	strain gauge	243–333 K	73–1499	Takagi et al. 2004
1,1,1-Trifluoroethane			mercury manometer	174–226 K	3.49–101.01	Russell et al. 1944
	299.995 K	1331	manometer/densimeter	278–340 K	769–3337	Widiatmo et al. 1994
	298.22 K	1265.1	isochoric	244–345 K	226–3717	Giuliani et al. 1995b
	300 K	1327.0	Burnett apparatus	295–342 K	1164–3474	Zhang et al. 1995a
	279.484 K	751.294	ebulliometry	236–279 K	160–751	Weber and Defibaugh 1996b
	298.165 K	1262.0	PVT apparatus	279–343 K	744–3556	Weber and Defibaugh 1996b
	293.149 K	1104.8		263–346 K	447–3763	Fujiwara et al. 1998
	283.11 K	834.8	VLE			Bobbo et al. 2000b
	298.16 K	1260.7	VLE			Bobbo et al. 2000b
	313.21 K	1832.5	VLE			Bobbo et al. 2000b
	300 K	1325.3	isochoric	300–345 K	1325–3748	Widiatmo et al. 2001
	298.16 K	1262.62	Burnett apparatus	251–343 K	292–3554	Duan et al. 2004
1,1,2,2-Tetrafluoroethane	299.994 K	546		200–390 K	15–4465	Maezawa et al. 1991b
1,1,1,2-Tetrafluoroethane	299.976 K	699		280–350 K	38–2459	Maezawa et al. 1990

	297.15 K	645.53		279–363 K	363–3236	Zhu et al. 1992
	298.21 K	666.7	isochoric	250–347 K	116–2316	Giuliani et al. 1995a
	298.13 K	666	acoustic interferometer	243–333 K	83–1673	Takagi 1996a
	293.66 K	580	VLE			Bobbo et al. 1998
	303.68 K	780.9	VLE			Bobbo et al. 1998
	283.62 K	420.7	VLE			Bobbo et al. 1998
	293.14 K	571.5		263–373 K	200–3973	Fujiwara et al. 1998
	293.15 K	571.3	VLE			Bobbo et al. 2001
	303.15 K	769.4	VLE			Bobbo et al. 2001
	313.15 K	1014.6	VLE			Bobbo et al. 2001
Pentafluoroethane			isochoric	195–339 K	20–100 bars	Wilson et al. 1992
			ebulliometry (glass)	219–247 K	74–262	Weber and Silva 1994
	284.714 K	951.5741	ebulliometry (metal)	240–285 K	200–952	Weber and Silva 1994
	299.985 K	1444	manometer/densimeter	220–335 K	79–3303	Widiatmo et al. 1994
	300 K	1446.6	Burnett apparatus	290–339 K	1107–3606	Ye et al. 1995
	298.21 K	1380	acoustic interferometer	242–333 K	221–3171	Takagi 1996b
	299.998 K	1447.57	isochoric	220–338 K	79–3529	Duarte-Garza et al. 1997b
	303.19 K	1568.5	VLE			Bobbo et al. 1999
	323.26 K	2539.3	VLE			Bobbo et al. 1999
	308.15 K	1778.8	VLE			Horstmann et al. 2004
Hexafluoroethane			calorimetry static	180–195 K	42–103	Pace and Aston 1948
	291.2 K	2902.1		177–291 K	35–2902	Kao and Miller 2000
1-Chloro-1,1-difluoroethane				320–400 K	632–3388	Maezawa et al. 1991a
	284.688 K	218.216	ebulliometry	225–285 K	15–218	Silva and Weber 1993
1-Chloro-1,2,2,2-tetrafluoroethane	286.098 K	258.829	ebulliometry (glass)	222–286 K	14–259	Weber and Silva 1994
1-Chloropentafluoroethane			calorimetry static	178–234 K	3–101	Aston et al. 1955
				178–346 K	3–2696	Mears et al. 1966
1,1-Dichloro-1-fluoroethane	300 K	84.20	Burnett apparatus	250–450 K	9–2791	Duarte-Garza et al. 1997a
	299.968 K	86		200–400 K	4–1177	Maezawa et al. 1991b
	299.795 K	83.43	comparative ebulliometry	271–313 K	25–129	Weber 1992
1,1-Dichlorotrifluoroethane	289.988 K	67		280–350 K	46–440	Maezawa et al. 1990
	308.26 K	131	isochoric	308–457 K	131–3658	Piao et al. 1991
	293.143 K	76.6	isochoric	243–448 K	7–3172	Oguchi et al. 1992
	299.950 K	97.45	comparative ebulliometry	272–308 K	30–130	Weber 1992
1,2-Dichloro-1,1,2,2-tetrafluoroethane			literature summary	–95.4–3.50°C	0.133–101.325	Stull 1947
1,1,1-Trichloro-2,2,2-trifluoroethane	298.2 K	48.143	isoteniscopic	287–309 K	31–72	Hiraoka and Hildebrand 1963
1,1,2-Trichloro-1,2,2-trifluoroethane	20.19°C	36.64	isoteniscopic	–8.4–210.62°C	10.08–3266.72	Benning and McHarness 1940
	30.2°C	53.329	literature summary	–68.0–47.6°C	0.133–101.325	Stull 1947

(Continued)

TABLE 5.1.5.3 *(Continued)*

Compound	Temp. °C or K	P^S kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
	298.2 K	48.476	isoteniscopic	273–318 K	17–97	Hiraoka and Hildebrand 1963
1,1,2,2-Tetrachloro-1,2-difluoroethane	20°C	6.106		10–92°C	4–101	Hovorka and Geiger 1933
	19.8°C	5.333	literature summary	–37.5–92.0°C	0.1333–101.325	Stull 1947
2-Fluoropropane	30°C	407	VLE			Parrish and Sitton 1982
	50°C	700	VLE			Parrish and Sitton 1982
1,1,2,2,3-Pentafluoropropane	298.98 K	100.7	isochoric	258–353 K	16–573	Di Nicola and Passerini 2002
1,1,1,3,3-Pentafluoropropane	298.17 K	151.9	isochoric	293–426 K	127–3595	Sotani & Kubota 1999
	298.21 K	149.04	Burnett apparatus	255–393 K	21–1951	Wang and Duan 2004
	293.15 K	122.8	VLE			Bobbo et al. 2001
	303.15 K	178.4	VLE			Bobbo et al. 2001
	313.15 K	250.8	VLE			Bobbo et al. 2001
	293.15 K	123.1	VLE			Bobbo et al. 2001
	303.15 K	178.1	VLE			Bobbo et al. 2001
	313.15 K	250.6	VLE			Bobbo et al. 2001
	297.97 K	147.1	isochoric	266–352 K	35–762	Di Nicola 2001
1,1,1,2,2-Pentafluoropropane	30°C	535.05	mercury piston gauge	–5.34–106.96°C	33.33–3137.4	Shank 1967
	292.955 K	397.36	comparative ebulliometry	248–326 K	74–995	Weber and Defibaugh 1996a
1,1,1,2,3,3-Hexafluoropropane	300 K	219.6	Burnett apparatus	300–410 K	220–3264	Zhang et al. 1995b
	283.12 K	118.6	VLE			Bobbo et al. 2000c
	298.16 K	205.8	VLE			Bobbo et al. 2000c
	313.21 K	340.4	VLE			Bobbo et al. 2000c
	283.12 K	118.4	VLE			Bobbo et al. 2000c
	298.17 K	207.0	VLE			Bobbo et al. 2000c
	313.22 K	338.5	VLE			Bobbo et al. 2000c
	298.41 K	208.1	isochoric	255–363 K	35–1266	Di Nicola and Giuliani 2000
1,1,1,3,3,3-Hexafluoropropane	299.15 K	281.15	Burnett apparatus	253–396 K	44–3064	Duan et al. 2004
	283.62 K	162.6	VLE			Bobbo et al. 1998
	303.68 K	325.8	VLE			Bobbo et al. 1998
	303.2 K	322.2	VLE			Bobbo et al. 1999
	323.26 K	584.2	VLE			Bobbo et al. 1999
	323.26 K	585.7	VLE			Bobbo et al. 1999
	298.27 K	272.5	isochoric	248–360 K	34–1472	Di Nicola et al. 1999
	283.13 K	160.0	VLE			Bobbo et al. 2000a
	303.19 K	322.3	VLE			Bobbo et al. 2000a

	323.26 K	586.3	VLE			Bobbo et al. 2000a
	283.11 K	160.9	VLE			Bobbo et al. 2000b
	298.16 K	272.5	VLE			Bobbo et al. 2000b
	313.21 K	439.3	VLE			Bobbo et al. 2000b
	283.12 K	159.1	VLE			Bobbo et al. 2000c
1,1,1,2,3,3,3-Heptafluoropropane				238–373 K	41–2831	Salvi-Narkhede et al. 1992
	299.06 K	467.35	Burnett apparatus	243–375 K	54–2936	Shi et al. 1999
				273–373 K	192–2818	Gruzdev et al. 2002
	298.152 K	441.234		233–375 K	32–2937	Hu et al. 2002
	295.27 K	416.1	isochoric	235–365 K	36–2402	Di Nicola 2003
	297.22 K	441.61	Burnett apparatus	253–373 K	87–2825	Wang and Duan 2004
Octafluoropropane	29.17°C	9.69 atm		–60.15 – 67.65°C	0.306–24.13 atm	Brown 1963
				182–237 K	3.29–106.47	Crowder et al. 1967
	50°C	1652	VLE			Leu and Robinson 1992
	65°C	2304	VLE			Leu and Robinson 1992
	70°C	2554	VLE			Leu and Robinson 1992
Trichlorotrifluoropropane				48 – 90°C	19–88	Varuschenko & Druzhinina 1972#
1-Chloro-2,2,2-trifluoropropane				29 – 68°C	19–88	Varuschenko & Druzhinina 1972#
Perfluorobutane	20°C	232.033	isoteniscopic	–28–90°C	35–1388	Fowler et al. 1947
			recirculating still	233–260 K	16–64	Simons and Mausteller 1952
	31.73°C	330.3		–40–110°C	17–2178	Brown and Mears 1958
Perfluorocyclobutane	17.70°C	249		–36–18°C	26–249	Whipple 1952
				–32–0°C	30–131	Furukava et al. 1954#
	22.53°C	288.76		–40–115°C	19–2778	Martin 1962
	293.21 K	265.2		234–387 K	20–2697	Kao and Miller 2000
Perfluoropentane	24.10°C	83.23	equilibrium still	10–65°C	46.34–318.84	Barber and Cady 1956
	297.59 K	84.71		221–303 K	1–104	Crowder et al. 1967
Perfluorocyclopentane	22.57°C	101.53	equilibrium still	17–56°C	82–307	Barber and Cady 1956
	296.83 K	105.72		230–297 K	2.60–105.72	Crowder et al. 1967
Perfluoro-2-methylcyclopentane	23.82°C	27.464	equilibrium still	4–68°C	11–143	Stiles and Cady 1952
	298.86 K	30.15		254–451 K	2.71–1763.46	Crowder et al. 1967
Perfluoro-3-methylcyclopentane	300.78 K	32.13		255–450 K	2.99–1674.8	Crowder et al. 1967
Perfluorocyclohexane				63–121°C	152–709	Rowlinson and Thacker 1957#
	300.74 K	33.75		253–451 K	2.11–2006.54	Crowder et al. 1967
Perfluorohexane	24.9°C	29.051	equilibrium still	11–69°C	15–149	Stiles and Cady 1952
	30.06°C	36.461	equilibrium still	30–57°C	36–102	Dunlap et al. 1958

(Continued)

TABLE 5.1.5.3 *(Continued)*

Compound	Temp. °C or K	P^S kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
	291.52 K	21.85		256–447 K	3.28–1701.14	Crowder et al. 1967
Fluoroalkenes						
Tetrafluoroethene				–131 – –65°C	1–177	Furukava et al. 1953#
Chlorotrifluoroethene			manometer	195–250 K	6–123	Booth et al. 1933
	21.9°C	577.55	manometer	21.9–107°C	577.55–3951.68	Booth and Swinehart 1935
			literature summary	–116 – –27.9°C	0.1333–101.325	Stull 1947
			calorimetry static	–67 – –11°C	13–205	Oliver et al. 1951
1,2-Dichloro-1,2-difluoroethene	295 K	105.8	manometer	240–295 K	8–106	Booth et al. 1933
	20.9°C	101.325	literature summary	–82.0–20.9°C	0.1333–101.325	Stull 1947
1,1-Dichloro-2,2-difluoroethene	295 K	105.8	manometer	240–295 K	8–106	Booth et al. 1933
Hexafluoropropene	19.75°C	652.7		–41–20°C	62–653	Whipple 1952

* VLE – vapor-liquid equilibrium.

** For temperature dependence equation, see reference.

Boublik et al. 1984.

TABLE 5.1.5.4
Henry's law constants and octanol-water partition coefficients for fluoroalkanes and fluoroalkenes

Compound	Henry's law constant Pa•m³/mol	Temp. °C	Method/temp. range	Reference	K_{OW}	Reference
Fluoroalkanes						
Fluoromethane	1418	25	calculated	Yaws et al. 1991	0.51	Sangster 1993
	1948	20		Glew & Moelwyn-Hughes 1953	0.51	Hansch et al. 1995
	1717	25	calculated C_A/C_W	Hine & Mookerjee 1975		
	1742	20T		Staudinger & Roberts 2001		
Difluoromethane	1160	25		Yaws et al. 1991	0.20	Sangster 1993, Hansch et al. 1995
Trifluoromethane	5907	25	gas stripping-GC	Warner et al. 1987	0.64	Hansch & Leo 1985
	9211	25		Hine & Mookerjee 1975	0.64	Sangster 1993
	7794	25		Yaws et al. 1991	0.64	Hansch et al. 1995
	9626	25	calculated-P/C	Howard 1993	0.64	Howard 1993, Hansch et al. 1995
Tetrafluoromethane	539961	25		Yaws et al. 1991	1.18	Sangster 1993, Hansch et al. 1995
Chlorofluoromethane	654.4	25		Yaws et al. 1991		
Dichlorofluoromethane	529.1	25		Yaws et al. 1991	1.55	Hansch et al. 1995
Chlorodifluoromethane	3058	25		Yaws et al. 1991	1.08	Hansch et al. 1995
	2979	25		Howard 1993	1.08	Howard 1993
Chlorotrifluoromethane	113889	25		Yaws et al. 1991	1.65	Hansch et al. 1995
Dichlorodifluoromethane	28704	19.93	0–40°C	Warner & Weiss 1985	2.16	Hansch et al. 1996
	39557	25		Yaws et al. 1991	2.16	Howard 1997
	27976	25		Howard 1997		
	26810	20T		Staudinger & Roberts 2001		
Trichlorofluoromethane	7925	19.93	0-40°C	Warner & Weiss 1985	2.53	Hansch et al. 1995
	10234	25T		Ashworth et al. 1988	2.53	Howard 1990
	9827	25		Howard 1990		
	12341	25		Yaws et al. 1991		
	7824	20T		Staudinger & Roberts 2001		
Fluoroethane	2253	25		Yaws et al. 1991		
1,1-Difluoroethane	2672	25		Yaws et al. 1991	0.75	Hansch et al. 1995
	2203	25		Hine & Mookerjee 1975	0.75	Sangster 1993
	2061			Howard 1993	0.75	Howard 1993

(Continued)

TABLE 5.1.5.4 *(Continued)*

Compound	Henry's law constant Pa•m³/mol	Temp. °C	Method/temp. range	Reference	K_{OW}	Reference
	1876	25		Zheng et al. 1997		
1,1,2-Trifluoroethane	32323	25T	EPICS-GC	Ashworth et al.1988		
	24616	20T		Staudinger & Roberts 2001		
1,1,1,2-Tetrafluoroethane	5629	25		Zheng et al. 1997	1.06	Franklin 1993
Hexafluoroethane	1715432	25		Yaws et al. 1991	2.00	Sangster 1993
	1652940	25T		Bonifacio et al. 2001	2.00	Hansch et al. 1995
1-Chloro-1,1-difluoroethane	24217	25	calc-bond contribution	Howard 1990	1.60	Howard 1990
1-Chloro-1,2,2,2-tetrafluoro-	54716	25		Howard 1997	1.867	estimated, Howard 1997
1-Chloropentafluoroethane	261418	25		Yaws et al. 1991	2.30	Howard 1997
	309041	25		Howard 1997		
1,1-Dichloro-1-fluoroethane	2442	25		Howard 1997	2.04	Howard 1997
1,2-Dichlorotetrafluoroethane	122502	25		Yaws et al. 1991	2.82	Sangster 1993, Hansch et al. 1995
1,1-Dichlorotetrafluoroethane					2.85	Sangster 1993, Hansch et al. 1995
1,1,2-Trichloro-1,2,2-trifluoro-	49132	25		Yaws et al. 1991	3.16	McDuffie 1981, Sangster 1993
	53297		calculated-P/C	Howard 1990	3.16	Howard 1990, Hansch 1995
1,1-Difluorotetrachloroethane	171239			Howard 1993	2.85	estimated, Howard 1993
1,2-Difluoro-1,1,2,2-tetrafluoro-	283710		calculated-P/C	Howard 1990	2.82	Howard 1990, Sangster 1993, Hansch et al. 1995
1,1,2,2-Tetrachloro-1,2-difluoro-	9869		calculated-C_A/C_W	Hine & Mookerjee 1975	3.73	Howard 1990
1-Fluoropropane	1627	14		Yaws et al. 1991		
2-Fluoropropane	1713	15		Yaws et al. 1991		
Perfluorocyclobutane	391925	25		Yaws et al. 1991		
Fluoroalkenes						
1,1-Difluoroethene	39344	25		Yaws et al. 1991	1.24	Hansch et al. 1995
Tetrafluoroethene	61981	25		Yaws et al. 1991		
Chlorotrifluoroethene	63328	25		Yaws et al. 1991		
Hexafluoropropene	349397	25		Wilhelm et al. 1977		

TABLE 5.1.5.5
Atmospheric fate rates for fluoroalkanes

	Atmospheric fate rate (photooxidation in air)				
Compound	**T/K**	**k_{OH}*/(cm^3 molecule^{-1} s^{-1})**	**Temp. range****	**Lifetime, τ**	**Reference**
Fluoroalkanes					
Fluoromethane	296	16×10^{-15}			Howard & Evenson 1976a
	298	1.68×10^{-14}	294–480 K		Atkinson 1989
				2–4.1 yr	Cooper et al. 1992
Difluoromethane	296	7.8×10^{-15}			Howard & Evenson 1976a
	298	7.2×10^{-15}	293–425 K		Clyne et al.1978
	298	1.09×10^{-14}	250–492 K		Atkinson 1989
	298	1.13×10^{-14}	222–381 K	7.1–7.7 yr	Talukdar et al. 1991
				4–7.3 yr	Cooper et al. 1992
Trifluoromethane	296	0.2×10^{-15}			Howard & Evenson 1976a
	298	2.4×10^{-16}	387–1445		Atkinson 1989
Tetrafluoromethane	298	$<4 \times 10^{-16}$			Atkinson 1989
Chlorofluoromethane	296	37×10^{-15}			Howard & Evenson 1976a
	298	4.41×10^{-14}	245–486 K		Atkinson 1989
Dichlorofluoromethane	296	26×10^{-15}			Howard & Evenson 1976a
	298	3.9×10^{-14}	293–425 K		Clyne et al. 1978
	298	3.03×10^{-14}	241–483 K		Atkinson 1989
Chlorodifluoromethane	296	3.4×10^{-15}			Howard & Evenson 1976a
	298	4.1×10^{-15}	293–425 K		Clyne et al. 1978
	298	4.68×10^{-15}	250–482 K		Atkinson 1989
				17.2 yr	Brown et al. 1990
Chlorotrifluoromethane	296	$<0.7 \times 10^{-15}$			Howard & Evenson 1976a
	298	$<7 \times 10^{-16}$			Atkinson 1989
Dichlorodifluoromethane	296	$<1.0 \times 10^{-15}$			Atkinson et al.1975
	296	$<0.4 \times 10^{-15}$			Howard & Evenson 1976a
	293	$<10^{-16}$		>330 yr	Cox et al. 1976
	298	$<1.0 \times 10^{-17}$			Atkinson 1989
				105 yr	Brown et al. 1990
Trichlorofluoromethane	296	$<1.0 \times 10^{-15}$			Atkinson et al. 1975
	296	$<0.5 \times 10^{-15}$			Howard & Evenson 1976a
	293	$<10^{-17}$		1000 yr	Cox et al. 1976
	298	$<1.0 \times 10^{-17}$			Atkinson 1989

(Continued)

TABLE 5.1.5.5 *(Continued)*

	Atmospheric fate rate (photooxidation in air)				
Compound	**T/K**	**k_{OH}*/(cm^3 molecule^{-1} s^{-1})**	**Temp. range****	**Lifetime, τ**	**Reference**
				60 yr	Brown et al. 1990
				182–635 yr	Cooper et al. 1992
Fluoroethane				0.2–1 yr	Cooper et al. 1992
1,1-Difluoroethane	298	5.1×10^{-14}	293–425 K		Clyne et al. 1978
	295	3.4×10^{-14}			Atkinson 1989
	303	5.6×10^{-14}	230–423 K	1.5 yr	Brown et al. 1990
	298	4.2×10^{-14}	243–400 K	1.5 yr	Liu et al. 1990
				1–1.68 yr	Cooper et al. 1992
1,2-Difluoroethane				0.58–0.8 yr	Cooper et al. 1992
1,1,1-Trifluoroethane	298	1.5×10^{-15}	293–425 K		Clyne et al. 1978
	298	1.35×10^{-15}	223–374	72–74 yr	Talukdar et al. 1991
				6.3 yr	Brown et al. 1990
				20–45 yr	Cooper et al. 1992
1,1,2-Trifluoroethane	298	4.9×10^{-14}	293–425		Clyne et al. 1978
				1–3.8 yr	Cooper et al. 1992
1,1,2,2-Tetrafluoroethane	298	6.9×10^{-15}	293–425		Clyne et al. 1978
	298	8.54×10^{-15}	249–473 K		Atkinson 1989
				2–12.3 yr	Cooper et al. 1992
1,1,1,2-Tetrafluoroethane	298	6.9×10^{-15}	293–425		Clyne et al. 1978
	301	6.9×10^{-15}	231–423 K	10.7 yr	Brown et al. 1990
	298	5.18×10^{-15}	243–400 K	14.4 yr	Liu et al. 1990
					Franklin 1993
				13.1–15.5 yr	Cooper et al. 1992
Pentafluoroethane	298	5.0×10^{-15}	293–425 K		Clyne et al. 1978
	303	2.9×10^{-15}	226–423 K	22.1 yr	
	298	1.9×10^{-15}	220–364 K	47–48 yr	Talukdar et al. 1991
				17–28.1 yr	Cooper et al. 1992
1-Chloro-1,1-difluoroethane	298	6.74×10^{-15}	293–425 K		Clyne et al. 1978
	298	3.58×10^{-15}	273–375 K		Atkinson 1989
	303	3.7×10^{-15}	231–423 K	15.4 yr	Brown et al. 1990
	298	4.02×10^{-15}	243–400 K	17.8 yr	Liu et al. 1990
1-Chloro-1,1,2-trifluoroethane	298	1.5×10^{-14}	293–425 K		Clyne et al. 1978
	298	1.61×10^{-14}	263–373 K		Atkinson 1989

1-Chloro-1,2,2,2-tetrafluoroethane	298	1.02×10^{-14}	250–375 K		Atkinson 1989
1,1-Dichloro-1-fluoroethane	298	7.1×10^{-15}	243–400 K	6.7 yr	Liu et al. 1990
	297	1.61×10^{-14}	238–426 K	4.3 yr	Brown et al. 1990
	298	5.92×10^{-15}	233–393 K	13–14 yr	Talukdar et al. 1991
1,2-Dichloro-1,1-difluoroethane	298	2.61×10^{-14}	249–473 K		Atkinson 1989
1,1-Dichlorotrifluoroethane	298	4.2×10^{-14}	293–425 K		Clyne et al. 1978
	298	3.34×10^{-14}	245–375 K		Atkinson 1989
	303	5.9×10^{-14}	232–425 K	1.0 yr	Brown et al. 1990
	298	3.52×10^{-14}	270–400 K	1.4 yr	Liu et al. 1990
1,1,2,2,3-Pentafluoropropane	298	2×10^{-14}, 4×10^{-14}		2, 1.3 yr	Cooper et al. 1993
1,1,1,2,2-Pentafluoropropane	298	7×10^{-15}, 8×10^{-15}		7 yr	Cooper et al. 1993
1,1,1,2,3,3-Hexafluoropropane	298	4×10^{-15}, 6×10^{-15}		10, 9 yr	Cooper et al. 1993
1,1,1,3,3,3-Hexafluoropropane	298	5×10^{-16}, 2×10^{-16}		77, 218 yr	Cooper et al. 1993
1,1,1,2,3,3,3-Heptafluoropropane	298	7×10^{-16}		63, 72 yr	Cooper et al. 1993

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* k_{OH} = second order reaction rate constant with hydroxyl radicals

** For temperature dependence equation, see reference.

TABLE 5.2.1
Summary of physical properties of halogenated hydrocarbons

							Molar volume, V_M cm^3/mol	
Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	MW/ρ at 20°C	Le Bas
Chloroalkanes:								
Chloromethane (Methyl chloride)	74-87-3	CH_3Cl	50.488	–97.7	–24.09	1	54.79	50.5
Dichloromethane	75-09-2	CH_2Cl_2	84.933	–97.2	40	1	64.07	71.4
Trichloromethane (Chloroform)	67-66-3	$CHCl_3$	119.378	–63.41	61.17	1	79.67	92.3
Tetrachloromethane (Carbon tetrachloride)	56-23-5	CCl_4	153.823	–22.62	76.8	1	96.50	113.2
Chloroethane (Ethyl chloride)	75-00-3	C_2H_5Cl	64.514	–138.4	12.3	1	72.00	72.7
1,1-Dichloroethane	75-34-3	$C_2H_4Cl_2$	98.959	–96.9	57.3	1	84.18	93.6
1,2-Dichloroethane	107-06-2	$C_2H_4Cl_2$	98.959	–35.7	85.3	1	79.04	93.6
1,1,1-Trichloroethane	71-55-6	$C_2H_3Cl_3$	133.404	–30.01	74.09	1	99.70	114.5
1,1,2-Trichloroethane	79-00-5	$C_2H_3Cl_3$	133.404	–36.3	113.8	1	92.69	114.5
1,1,1,2-Tetrachloroethane	630-20-6	$C_2H_2Cl_4$	167.849	–70.2	130.2	1	108.95	135.4
1,1,2,2-Tetrachloroethane	79-34-5	$C_2H_2Cl_4$	167.849	–42.4	145.2	1	105.27	135.4
Pentachloroethane	76-01-7	C_2HCl_5	202.294	–28.78	162.0	1	120.36	156.3
Hexachloroethane	67-72-1	C_2Cl_6	236.739				113.22	177.2
1-Chloropropane (*n*-Propyl chloride)	540-54-5	C_3H_7Cl	78.541	–122.9	46.5	1	88.26	94.9
2-Chloropropane	75-29-6	C_3H_7Cl	78.541	–117.18	35.7	1	91.15	94.9
1,2-Dichloropropane	78-87-5	$C_3H_6CL_2$	112.986	–100.53	96.4	1	97.74	115.8
1,2,3-Trichloropropane	96-18-4	$C_3H_5Cl_3$	147.431	–14.7	157	1	106.59	136.7
1-Chlorobutane (*n*-Butyl chloride)	109-69-3	C_4H_9Cl	92.567	–123.1	78.4	1	104.51	117.1
2-Chlorobutane	78-86-4	C_4H_9Cl	92.567	–131.3	68.2	1	106.01	117.1
1-Chloropentane (*n*-Amyl chloride)	543-59-6	$C_5H_{11}Cl$	106.594	–99.0	108.4	1	120.85	139.3
1-Chlorohexane	544–10–5	$C_6H_{13}Cl$	120.620	–94.0	135.1	1	137.30	161.5
1-Chloroheptane	629–06–1	$C_7H_{15}Cl$	134.647	–69.5	160.4	1	153.74	183.7
1-Chlorooctane	111–85–3	$C_8H_{17}Cl$	148.674	–57.8	183.5	1	170.15	205.9
1-Chlorononane	2473–01–0	$C_9H_{19}Cl$	162.700	–39.4	205.2	1	206.31	228.1
1-Chlorodecane	1002–69–3	$C_{10}H_{21}Cl$	176.727	–31.3	225.9	1	203.02	250.3

Chloroalkenes:								
Chloroethene (Vinyl chloride)	75-01-4	C_2H_3Cl	62.498	–153.84	–13.8	1	68.63	65.3
1,1-Dichloroethene	75-35-4	$C_2H_2Cl_2$	96.943	–122.56	31.6	1	79.91	86.2
cis-1,2-Dichloroethene	156-59-2	$C_2H_2Cl_2$	96.943	–80.0	60.1	1	75.52	86.2
trans-1,2-Dichloroethene	156-60-5	$C_2H_2Cl_2$	96.943	–49.8	48.7	1	77.15	86.2
Trichloroethylene	79-01-6	C_2HCl_3	131.388	–84.7	87.21	1	89.73	107.1
Tetrachloroethylene	127-18-4	C_2Cl_4	165.833	–22.3	121.3	1	120.19	128.0
cis-1,3-Dichloropropene	10061–01–5	$C_3H_4Cl_2$	110.970		104.3		91.18	108.4
trans-1,3-Dichloropropene	10061–02–6	$C_3H_4Cl_2$	110.970		112		90.66	108.4
Chloroprene	126-99-8	C_4H_5Cl	88.536	–130	59.4	1	92.39	102.3
Hexachloro-1,3-butadiene	87-68-3	C_4Cl_6	260.761	–21	215	1	155.03	206.8
Hexachlorocyclopentadiene	77-47-4	C_5H_6	272.772	–9	239	1	160.27	210.1
Bromoalkanes and bromoalkenes:								
Bromomethane	74-83-9	CH_3Br	94.939	–93.68	3.5	1	56.66	52.9
Dibromomethane	74-95-3	CH_2Br_2	173.835	–52.5	97	1	69.62	76.2
Tribromomethane	75-25-2	$CHBr_3$	252.731	8.69	149.1	1	87.42	99.5
Bromoethane (Ethyl bromide)	74-96-4	C_2H_5Br	108.965	–118.6	38.5	1	75.12	75.1
1,2-Dibromoethane	106-93-4	$C_2H_4Br_2$	187.861	9.84	131.6	1	86.21	98.4
1-Bromopropane (*n*-Propyl bromide)	106-94-5	C_3H_7Br	122.992	–110.3	71.1	1	90.86	97.3
2-Bromopropane	75-26-3	C_3H_7Br	122.992	–89.0	59.5	1	93.60	97.3
1,2-Dibromopropane	78-75-1	$C_3H_6Br_2$	201.888	–55.49	141.9	1	104.48	120.6
1-Bromobutane (*n*-Butyl bromide)	109-65-9	C_4H_9Br	137.018	–112.6	101.6	1	107.40	119.5
1-Bromopentane (*n*-Amyl bromide)	110–53–2	$C_5H_{11}Br$	151.045	–88.0	129.8	1	123.99	141.7
1-Bromohexane	111–25–1	$C_6H_{13}Br$	165.071	–83.7	155.3	1	140.56	163.9
1-Bromoheptane	629–04–9	$C_7H_{15}Br$	179.098	–56.1	178.9	1	157.10	186.1
1-Bromooctane	111–83–1	$C_8H_{17}Br$	193.125	–55.0	200.8	1	173.64	208.3
1-Bromodecane	112–29–8	$C_{10}H_{21}Br$	221.178	–29.2	240.6	1	206.67	252.7
1-Bromododecane	143–15–7	$C_{12}H_{25}Br$	249.231	–9.5	276	1	239.67	297.1
Bromocyclohexane	108–85–0	$C_6H_{11}Br$	163.055	–56.5	166.2	1	122.06	141.5
Vinyl bromide	593–60–2	C_2H_3Br	106.949	–139.54	15.8	1	71.62	67.7

(*Continued*)

TABLE 5.2.1 (*Continued*)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol	
							MW/ρ at 20°C	Le Bas
Iodoalkanes:								
Iodomethane (Methyl iodide)	74-88-4	CH_3I	141.939	–66.4	42.43	1	62.28	62.9
Iodoethane (Ethyl iodide)	75-03-6	C_2H_5I	155.965	–111.1	72.3	1	80.57	85.1
1-Iodopropane (*n*-Propyl iodide)	107-08-4	C_3H_7I	169.992	–101.3	102.5	1	97.20	107.3
2-Iodopropane	75–30–9	C_3H_7I	169.992	–90	89.5	1	99.75	107.3
1-Iodobutane (*n*-Butyl iodide)	542-69-8	C_4H_9I	184.018	–103	130.5	1	113.91	129.5
1-Iodopentane	628–17–1	$C_5H_{11}I$	198.045	–85.6	157.0	1	130.63	151.7
Mixed halogenated hydrocarbons:								
Bromochloromethane	74-97-5	CH_2BrCl	129.384	–87.9	68.0	1	66.89	73.8
Bromodichloromethane	75-27-4	$CHBrCl_2$	163.829	–57	90	1	83.12	94.7
Dibromochloromethane	124-48-1	$CHBr_2Cl$	208.280	–20	120	1	84.98	97.1
Chlorodifluoromethane (HCFC-22)	75-45-6	$CHClF_2$	86.469	–157.42	–40.7	1	71.25	60.5
Dichlorodifluoromethane (CFC-12)	75-71-8	CCl_2F_2	120.914	–158	–29.8	1	90.97	81.4
Trichlorofluoromethane (CFC-11)	75-69-4	CCl_3F	137.368	–110.44	23.7	1	92.32	97.3
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	76-13-1	$C_2F_3Cl_3$	187.375	–36.22	47.7	1	119.84	129.5
1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112)	76–12–0	$C_2F_2Cl_4$	203.830	24.8	92.8	1		145.4

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 5.2.2
Summary of selected physical-chemical properties of halogenated hydrocarbons at 25°C

	Selected properties						Henry's law constant	
	Vapor pressure		Solubility				H/(Pa·m^3/mol)	
Compound	P^S/Pa	P_L/Pa	S/(g/m^3)	C^S/(mol/m^3)	C_L/(mol/m^3)	log K_{OW}	calcd P/C	exptl
Chloroalkanes:								
Chloromethane	570000	570000	5325	105.5	105.5	0.91	960.7*	894
Dichloromethane	58000	58000	13200	155.4	155.4	1.25	373.2	300
Trichloromethane	26200	26200	8200	68.69	68.69	1.97	381.4	427
Tetrachloromethane	15250	15250	800	5.200	5.200	2.83	2932	2989
Chloroethane	16000	16000	5700	88.35	88.35	1.43	181.1	1023
1,1-Dichloroethane	30260	30260	5040	50.93	50.93	1.79	594.1	569
1,2-Dichloroethane	10540	10540	8600	86.90	86.90	1.48	121.3	143
1,1,1-Trichloroethane	16500	16500	1290	9.670	9.670	2.49	1706	1763
1,1,2-Trichloroethane	3220	3220	4590	34.41	34.41	2.38	93.59	92.2
1,1,1,2-Tetrachloroethane	1580	1580	1070	6.375	6.375		247.8	
1,1,2,2-Tetrachloroethane	793	793	2830	16.86	16.86	2.39	47.03	25.7
Pentachloroethane	590	590	490	2.422	2.422	3.22	243.6	
Hexachloroethane	50	1923	50	0.2112	8.123	4.14	236.7	846
1-Chloropropane	46000	46000	2500	31.83	31.83	2.04	1445	
2-Chloropropane	68700	68700	3000	38.20	38.20	1.90	1798	
1,2-Dichloropropane	6620	6620	2740	24.25	24.25	2.00	273.0	287
1,2,3-Trichloropropane	492	492	1896	12.86	12.86		38.26	
1-Chlorobutane	13700	13700	615	6.644	6.644	2.64	2062	1537
2-Chlorobutane	20210	20210	1000	10.80	10.80		1871	2267
1-Chloropentane	4142	4142	198	1.858	1.858		2230	2375
Chloroalkenes:								
Chloroethene	354600	354600	2763	44.21	44.21	1.38	8021	2685
1,1-Dichloroethene	80500	80500	3344	34.49	34.49	2.13	2334	2624
cis-1,2-Dichloroethene	27000	27000	3500	36.10	36.10	1.86	747.8	460
trans-1,2-Dichloroethene	44400	44400	6260	64.57	64.57	1.93	687.6	958
Trichloroethylene	9900	9900	1100	8.372	8.372	2.53	1182	1034
Tetrachloroethylene	2415	2415	150	0.904	0.904	2.88	2670	1733

(Continued)

TABLE 5.2.2 (*Continued*)

	Selected properties						Henry's law constant	
	Vapor pressure		Solubility				H/(Pa·m^3/mol)	
Compound	P^S/Pa	P_L/Pa	S/(g/m^3)	C^S/(mol/m^3)	C_L/(mol/m^3)	log K_{OW}	calcd P/C	exptl
1,3-Dichloropropene						1.98		
Chloroprene	23194	23194				2.03		
Hexachloro-1,3-butadiene	20.0	20.0	3.2	0.013	0.013	4.70	1630	
Hexachlorocyclopentadiene	10.9	10.9	1.80	0.0066	0.0066	5.04	1652	
Bromoalkanes and bromoalkenes:								
Bromomethane	217700	217700	15223	160.3	160.3	1.19	631.9*	
Dibromomethane	6034	6034	11442	65.82	65.82	2.50	91.67	86.13
Tribromomethane	727	727	3100	12.27	12.27	2.38	59.27	46.61
Bromoethane	62500	62500	8939	82.04	82.04	1.6	1235*	
1,2-Dibromoethane	1500	1500	4152	22.10	22.10		67.87	65.86
1-Bromopropane	18440	18440	598	4.862	4.862	2.1	3792	
2-Bromopropane	31940	31940	3086	25.09	25.09	1.9	1273	
1,2-Dibromopropane	1040	1040	1428	7.073	7.073		147.0	
1-Bromobutane	5500	5500				2.6		
Vinyl bromide	140476	140476						
Iodoalkanes:								
Iodomethane	54000	54000	13894	97.89	97.89	1.5	551.6	541
Iodoethane	18160	18160	4041	25.91	25.91	2	700.9	
1-Iodopropane	5745	5745	1051	6.183	6.183	2.5	929.2	
1-Iodobutane	1848	1848	182	0.989	0.989	3	1868	
Mixed halogenated hydrocarbons:								
Bromochloromethane	19600	19600	14778	114.2	114.2	1.41	171.6	
Bromodichloromethane	6670	6670	4500	27.47	27.47	2.1	242.8	162
Dibromochloromethane			4000	19.20	19.20	2.24		86.13
Chlorodifluoromethane (HCFC-22)	1044000	1044000	2899	33.53	33.53		3022*	
Dichlorodifluoromethane (CFC-12)	651000	651000	300	2.481	2.481	2.16	40840*	
Trichlorofluoromethane (CFC-11)	102200	102200	1080	7.862	7.862	2.53	12890*	10243
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	48320	48320	166	0.886	0.886	3.16	114375*	32323

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H (Pa·m^3/mol) = 101325 Pa/C^S mol/m^3.

TABLE 5.2.3
Suggested half-life classes of halogenated hydrocarbons in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Cycloalkanes and cycloalkenes:				
Dichloromethane	6	6	7	8
Trichloromethane	6	6	7	8
Tetrachloroethane	8	6	7	8
Chloroethane	6	6	7	8
1,2-Dichloroethane	6	6	7	8
1,1,2,2-Tetrachloroethane	8	6	7	8
Pentachloroethane	8	6	7	8
Hexachloroethane	8	6	7	8
1,2-Dichloropropane	5	6	7	8
1,2,3-Trichloropropane	5	6	7	8
Chloroethene (Vinyl chloride)	3	5	6	7
Trichloroethylene	4	6	7	8
Tetrachloroethylene	5	6	7	8
Chloroprene	3	5	6	7
Bromoalkanes and bromoalkenes:				
Tribromomethane	6	6	7	8
Mixed halogenated hydrocarbons:	5	5	6	7
Bromodichloromethane	5	5	6	7
Trichlorofluoromethane (CFC-11)	8	8	9	9

Class	Mean half-life (h)	Range (h)
1	5	< 10
2	17 (~ 1 d)	10–30
3	55 (~ 2 d)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 yr)	10,000–30,000
9	55000 (~ 6 yr)	> 30,000

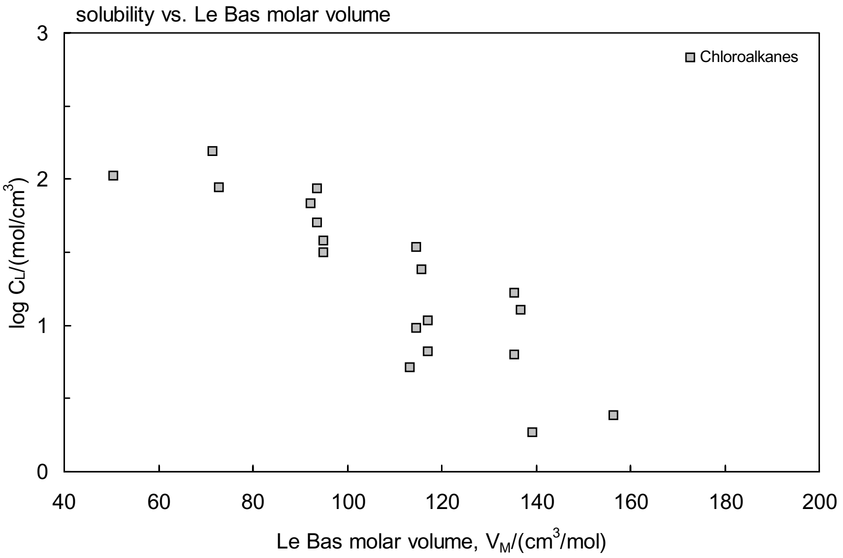

FIGURE 5.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for chloroalkanes.

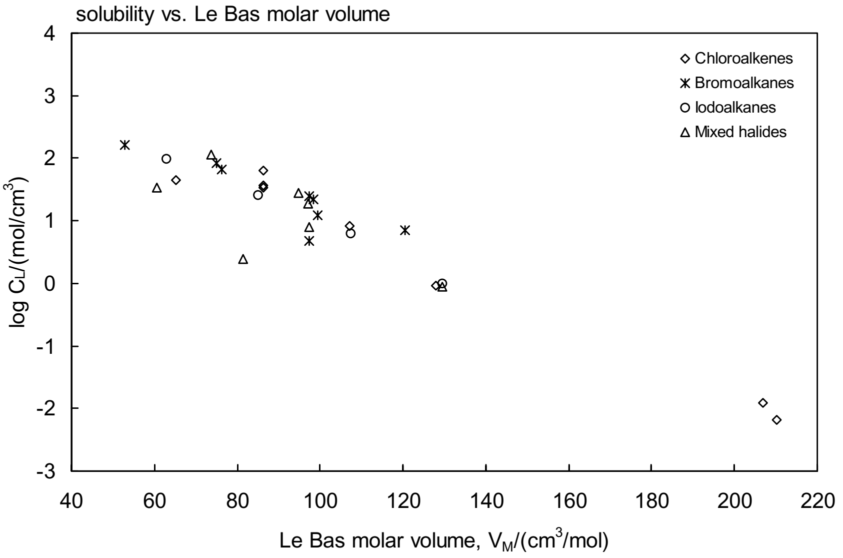

FIGURE 5.2.2 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

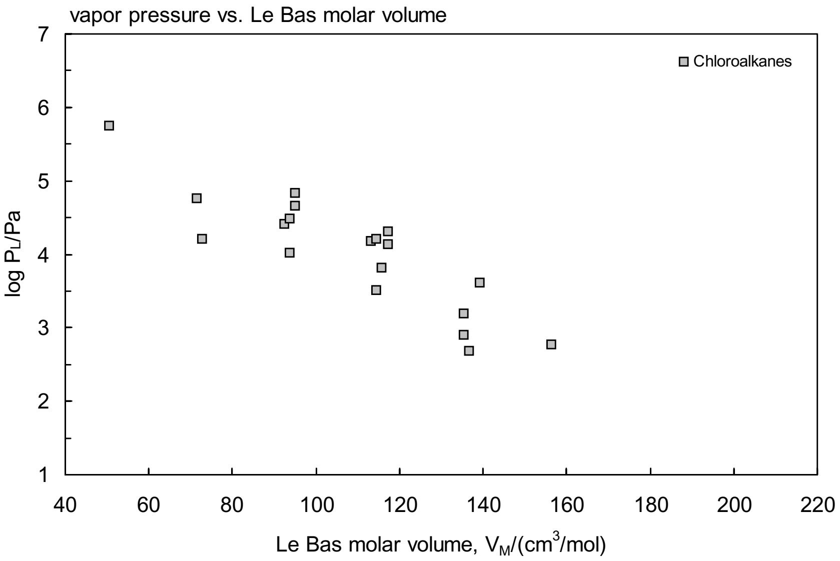

FIGURE 5.2.3 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for chloroalkanes.

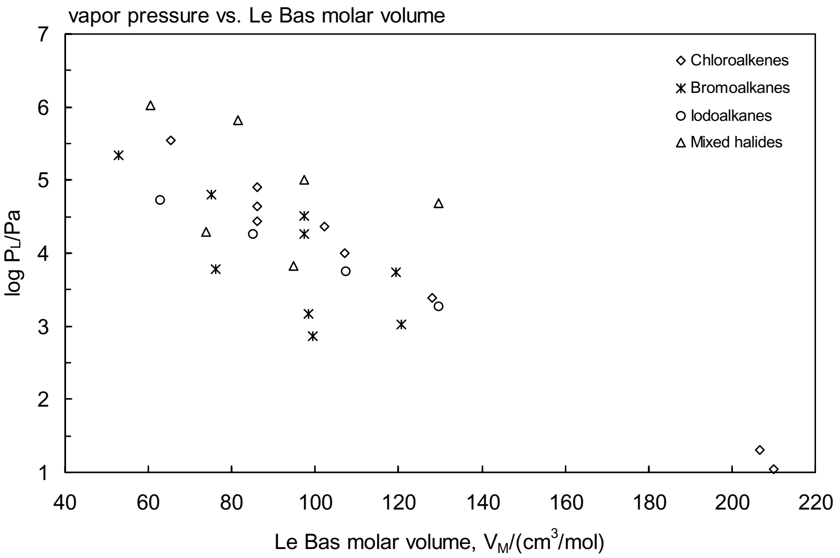

FIGURE 5.2.4 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

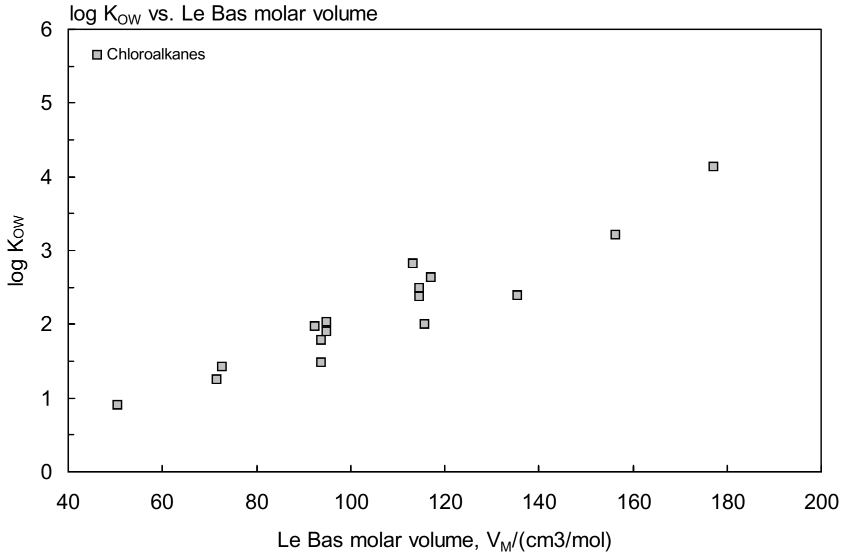

FIGURE 5.2.5 Octanol-water partition coefficient versus Le Bas molar volume for chloroalkanes.

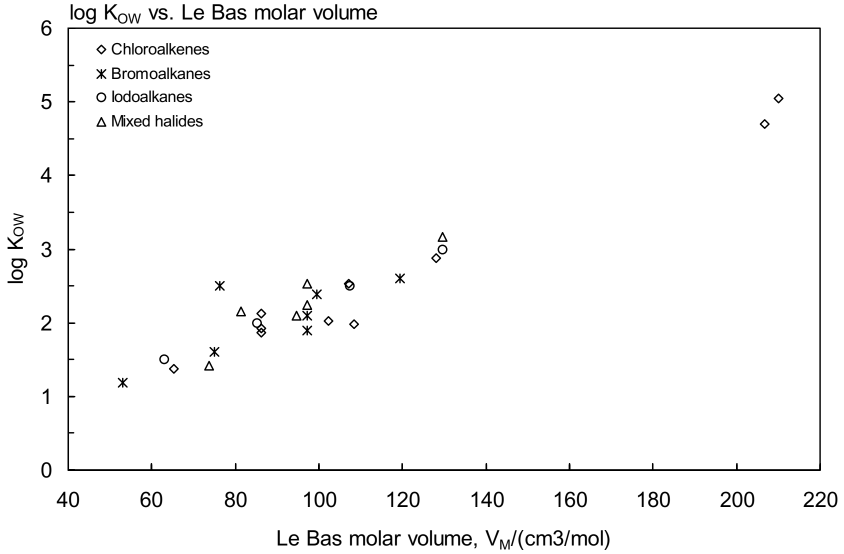

FIGURE 5.2.6 Octanol-water partition coefficient versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

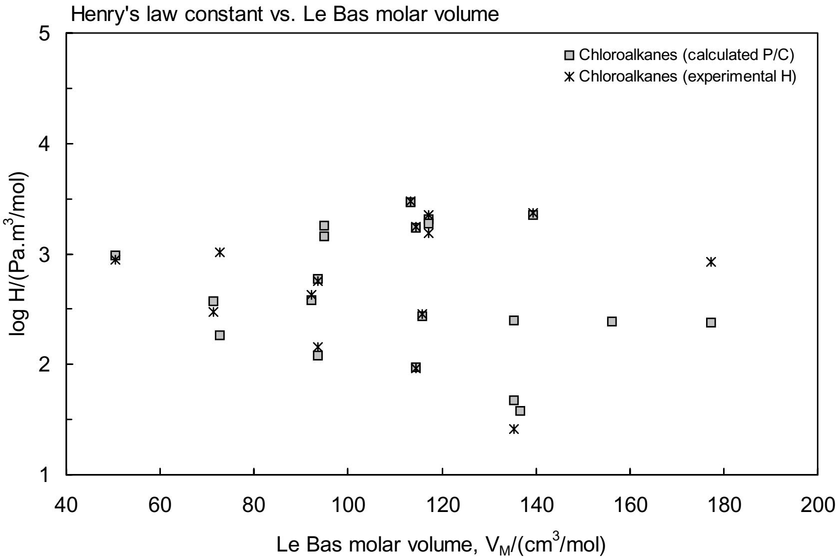

FIGURE 5.2.7 Henry's law constant versus Le Bas molar volume for chloroalkanes.

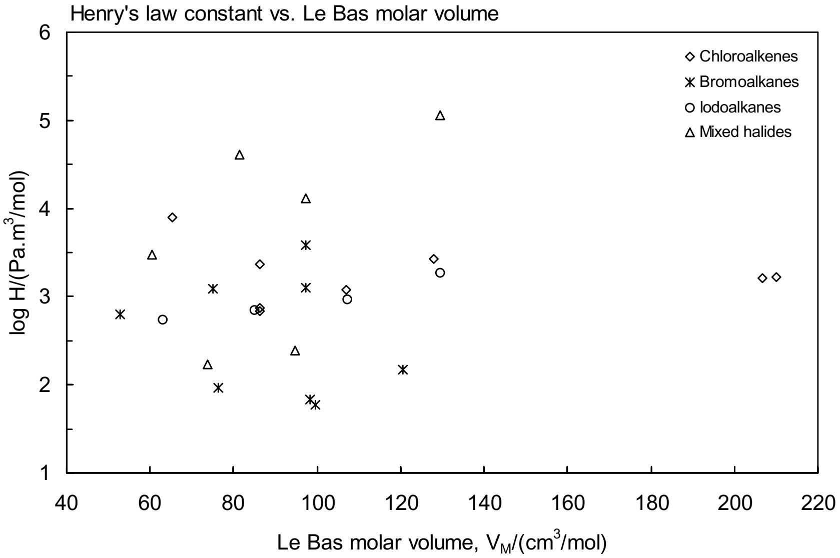

FIGURE 5.2.8 Henry's law constant versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

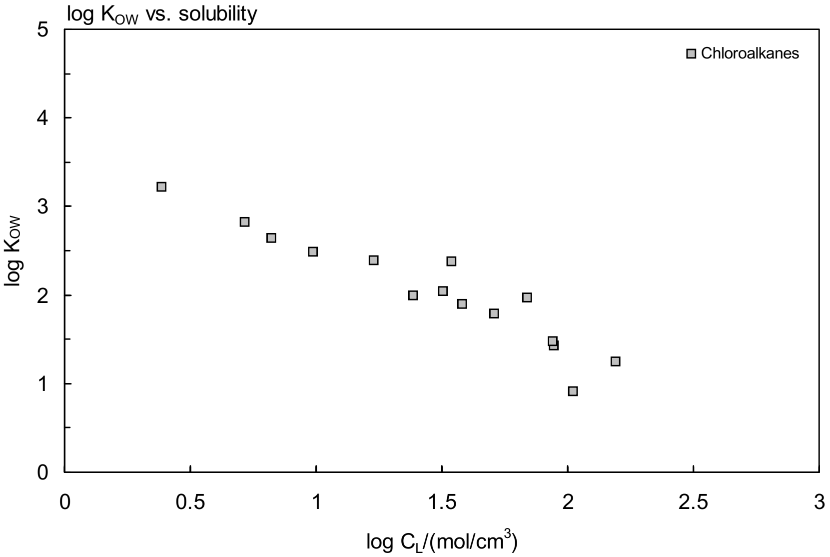

FIGURE 5.2.9 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for chloroalkanes.

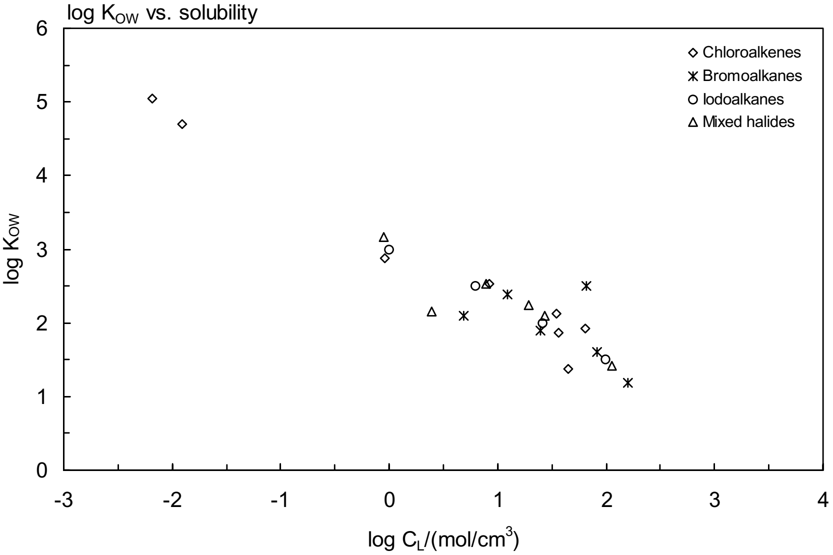

FIGURE 5.2.10 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for halogenated aliphatic hydrocarbons.

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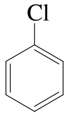
6 Chlorobenzenes and Other Halogenated Mononuclear Aromatics

CONTENTS

6.1 LIST OF CHEMICALS AND DATA COMPILATIONS

6.1.1 CHLOROBENZENES

6.1.1.1 Chlorobenzene



Common Name: Chlorobenzene
Synonym: monochlorobenzene, benzene chloride, phenyl chloride
Chemical Name: chlorobenzene
CAS Registry No: 108-90-7
Molecular Formula: C_6H_5Cl
Molecular Weight: 112.557
Melting Point (°C):
 –45.31 (Lide 2003)
Boiling Point (°C):
 131.72 (Lide 2003)
Density (g/cm^3 at 20°C):
 1.1058 (Weast 1972–73; Lide 2003)
Molar Volume (cm^3/mol):
 101.8 (20°C, calculated-density)
 116.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 9.49 (Dean 1985)
 11.88 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 488 (30°C, shake flask-interferometer, Gross & Saylor 1931)
 551 (Landolt-Börnstein 1951)
 488 (Seidell 1941)
 < 200 (residue-volume method, Booth & Everson 1948)
 500 (shake flask-UV, Andrews & Keefer 1950)
 490* (30°C, shake flask, Kisarov 1962)
 546, 523; 534 (21°C, generator column-GC; mean value, Chey & Calder 1972)
 463 (shake flask-UV, Vesala 1974)
 100 (Stephen & Stephen 1963)
 106.8* (shake flask-GC, measured range 5–45°C, Nelson & Smit 1978)
 472 (shake flask-GC, Aquan-Yuen et al. 1979)
 472 (shake flask-GC, Mackay et al. 1979, 1980, 1982b)
 503 (shake flask-UV, Yalkowsky et al. 1979)
 420, 450* (20°C; elution chromatography, UV adsorption, measured range 10–30°C, Schwarz & Miller 1980)
 295 (generator column-HPLC/UV, Tewari et al. 1982)
 498 (recommended, Horvath 1982)
 499 (generator column-HPLC/UV, Wasik et al. 1983)
 508 (HPLC-k′ correlation, converted from reported γ_W, Hafkenscheid & Tomlinson 1983a)
 295 (generator column-GC, Miller et al. 1984, 1985)
 495* (recommended, temp range 10–70°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(g/kg) = 11.3351 - 3.0290 \times 10^{-2}\cdot(T/K) - 1.8716 \times 10^{-4}\cdot(T/K)^2 + 0.559466 \times 10^{-6}\cdot(T/K)^3$; temp range 283–363 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)
490 (30°C, quoted, Dean 1985)
502 (shake flask-HPLC/UV, Banerjee 1984)
348 (shake flask-radiometric method, Lo et al. 1986)
428 (vapor phase saturation-GC, temp range 15–45°C, Sanemasa et al. 1987)
482* (20°C vapor-liquid equilibrium-activity coefficient, measured range 20–50°C, Cooling et al. 1992)
477 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
333 (shake flask-GC, Boyd et al. 1998)
496 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
$\ln x = -41.9062 + 6054.03/(T/K) + 1.3692 \times 10^{-4}\cdot(T/K)^2$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
470* (shake flask-GC, measured range 5–45°C, Ma et al. 2001)
426, 427, 511 (5, 15, 35°C, estimated-RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
1333* (22.2°C, summary of literature data, temp range –13.0 to 132.2°C, Stull 1947)
$\log (P/mmHg) = 7.18473 - 1556.6/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
$\log (P/mmHg) = 6.94504 - 1413.12/(216.0 + t/°C)$; temp range 40–200°C (Antoine eq. for liquid state, Dreisbach 1955)
7605* (56.28°C, ebulliometry, measured range 56.28–131.70°C, Dreisbach & Shrader 1949)
9657* (62.04°C, ebulliometry, measured range 62.04–131.7°C, Brown 1952)
1580 (interpolated-Antoine eq., Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 10098.0/(T/K)] + 8.5000$; temp range –35 to –15°C (Antoine eq., Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 9067.3/(T/K)] + 7.717535$; temp range –13 to 249.8°C (Antoine eq., Weast 1972–73)
1596, 1610 (extrapolated-Antoine eq., Boublik et al. 1973; 1984)
$\log (P/kPa) = 6.10416 - 1431.813/(217.655 + t/°C)$; temp range 62.04–131.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (P/kPa) = 6.07963 - 1419.045/(216.633 + t/°C)$; temp range 56.2–131.7°C (Antoine eq. from reported exptl. data of Derisbach & Shrader 1949, Boublik et al. 1984)
1586 (Daubert & Danner 1985)
1596 (extrapolated, Antoine eq., Dean 1985)
$\log (P/mmHg) = 6.97808 - 1431.05/(217.65 + t/°C)$; temp range 62–131.7°C (Antoine eq., Dean 1985, 1992)
1600 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.11512 - 1438.86/(-54.72 + T/K)$; temp range 333–405 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.62988 - 1897.41/(5.21 + T/K)$; temp range 405–597 K (Antoine eq.-II, Stephenson & Malanowski 1987)
1410* (gas saturation-GC, measured range –14.2 to 40°C, Liu & Dickhut 1994)
1828; 1560 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
$\log (P/mmHg) = 19.4343 - 2.5801 \times 10^3/(T/K) - 3.9391\cdot\log (T/K) - 4.4005 \times 10^{-11}\cdot(T/K) + 4.9583 \times 10^{-7}\cdot(T/K)^2$; temp range 228–632 K (Yaws 1994)
$\log P/kPa = 6.11512 - 1438.86/(T/K - 54.72)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
451 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
441 (calculated-bond contribution, Hine & Mookerjee 1975)
382 (batch stripping-GC, Mackay et al. 1979)
379 (calculated P/C, Mackay et al. 1979)
330* (equilibrium cell-concentration ratio, measured range 1.0–23.0°C, Leighton & Calo 1981)
$\ln (k_H/atm) = 16.83 - 3466/(T/K)$; temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
314 (batch air stripping-GC, Mackay & Shiu 1981)

398 (gas stripping-GC, Warner et al. 1987)
319 (20°C, EPICS-GC, Yurteri et al. 1987)
273 (20°C, calculated-P/C, Yurteri et al. 1987)
365* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 3.469 – 2689/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
460 (computer value, Yaws et al. 1991)
324* (extrapolated from equilibrium headspace-GC data, measured range 45–80°C, Ettre et al. 1993)
log (1/K_{AW}) = –2.9050240 + 1129.8083/(T/K); temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)
288 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
315 (gas stripping-GC, Shiu & Mackay 1997)
293 (headspace equilibrium-GC, de Wolf & Lieder 1998)
277.2 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
537 (modified EPICS method-GC, Ryu & Park 1999)
297 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 4.225 – 1507/(T/K) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
384* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
ln K_{AW} = 10.04 – 3359.7/(T/K); temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.84 (Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1985)
2.81 (calculated-fragment constant, Rekker 1977)
2.18 (^{14}C- LSC, Lu & Metcalf 1975)
2.84, 2.46, 2.18 (Hansch & Leo 1979)
2.79 (HPLC-RT correlation, Veith et al. 1979b)
2.84 (HPLC-k′ correlation, Könemann et al. 1979)
2.80 (HPLC-k′ correlation, Hanai et al. 1981)
2.81 (HPLC-k′ correlation, D'Amboise & Hanai 1982)
2.83 (shake flask-HPLC, Hammers et al. 1982)
2.18 (HPLC-k′ correlation, Miyake & Terada 1982)
2.80 (HPLC-k′ correlation, Hafkenscheid & Tomlinson 1983a)
2.98 (generator column-HPLC/UV, Wasik et al. 1983)
2.98 (generator column-GC/ECD, Miller et al. 1984; 1985)
2.81–2.84 (HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)
2.49 (HPLC-k′ correlation, Haky & Young 1984)
3.00 (HPLC-k′ correlation, De Kock & Lord 1987)
2.898 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
2.784 ± 0.061, 2.898 ± 0.004 (shake flask methods, interlaboratory studies, Brooks et al. 1990)
2.65, 2.73; 2.84 (25°C, 60°C, shake flask-UV/VIS; quoted lit. at 25°C, Kramer & Henze 1990)
2.86, 3.02 (centrifugal partition chromatography, Gluck & Martin 1990)
2.84 (recommended, Sangster 1993)
2.89 (recommended, Hansch et al. 1995)
2.98 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
2.96 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrăder 1999)
3.05* (estimated-RP-HPLC-k′ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

3.45* (20°C, HPLC-k′ correlation, measured range 10–50°C, Su et al. 2002)
log K_{OA} = 43910/(2.303·RT) – 4.107; temp range 10–50°C (HPLC-k′ correlation, Su et al. 2002)

Bioconcentration Factor, log BCF:

2.65 (fathead minnow, Veith et al. 1979b, 1980)
1.30 (Kenaga 1980a)

1.08 (fish, flowing water, Kenaga & Goring 1980)
2.21 (microorganisms-water, Mabey et al. 1982)
1.70 (algae, Freitag et al. 1984, 1985; Halfon & Reggiani 1986)
1.88 (fish, Freitag et al. 1984; Halfon & Reggiani 1986)
3.23 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
1.85 (fish, Freitag et al. 1985)
3.23 (activated sludge, Freitag et al. 1985)
1.93 (fish, calculated, Figueroa & Simmons 1991)

Sorption Partition Coefficient, log K_{OC}:
2.52 (sediment, Mabey et al. 1982)
2.18 (Kenaga 1980a)
2.59 (field data, Roberts et al. 1980; Schwarzenbach & Westall 1981; quoted, Voice & Weber 1985)
1.84 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
1.73–2.99 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
2.44, 2.50 (calculated from K_{OW}, Schwarzenbach & Westall 1981)
2.73 (soil, calculated-K_{OW}, Calamari et al. 1983)
2.10 (calculated-MCI χ, Koch 1983)
2.92 (calculated-K_{OW}, Yoshida et al. 1983b)
2.60 (Offshore Grand Haven sediment, batch equilibrium-sorption isotherm, Voice & Weber, Jr. 1985)
2.44 (calculated-MCI χ, Bahnick & Doucette 1988)
1.92–2.59 (soil, Howard 1989)
2.50; 2.17 (Captina silt loam, OC 1.49%, pH 4.17; McLaurin sandy loam, OC 0.66%, pH 4.42, batch equilibrium-sorption isotherm, Walton et al. 1992)
2.34 (calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.19, 2.20 (RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
1.97, 2.14, 1.77 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:
1.68 (Woodburn soil, organic matter 1.9%, batch equilibrium-sorption isotherm-GC/ECD, Chiou et al. 1983)
2.10, 2.32 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: estimated $t_{½}$ ~ 1–12 h from a flowing stream (Cadena, 1984; selected, Howard 1989);
$k = 0.033\ d^{-1}$ with $t_{½}$ = 21 d in spring at 8–16°C, $k = 0.152\ d^{-1}$ with $t_{½}$ = 4.6 d in summer at 20–22°C, $k = 0.053\ d^{-1}$ with $t_{½}$ = 13 d in winter at 3–7°C for periods when volatilization appears to dominate, and $k = 0.08\ d^{-1}$ with $t_{½}$ = 8.9 d with $HgCl_2$ in September 9–15, 1980 in marine mesocosm experiments; estimated half-lives from soil: $t_{½}$ = 0.3 d of 1-cm depth and $t_{½}$ = 12.6 d for 10 cm depth (Wakeham et al. 1983).
Photolysis: not environmentally significant or relevant (Mabey et al. 1982);
photolysis $k = 1.1 \times 10^{-5}\ d^{-1}$ with an estimated $t_{½}$ ~170 yr by sunlight in surface water at 40°N in the summer (Dulin et al. 1986)
$t_{½}$ = 21 d under sunlight in water (Mansour & Feicht 1994).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
photooxidation $t_{½}$ = 1553–62106 h in water, based on a measured rate for hydroxy radicals in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)
$k_{OH} = 9.0 \times 10^{-13}\ cm^3\ molecule^{-1}\ s^{-1}$, residence time of 13 d, loss of 7.4% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)
$k << 360\ M^{-1}\ h^{-1}$ for singlet oxygen and $k << 1\ M^{-1}\ h^{-1}$ for RO_2 radical (Mabey et al. 1982)
$k = (0.75 \pm 0.2)3\ M^{-1}\ s^{-1}$ for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k = 2.88 \times 10^{-3}$ h^{-1} in air (Yoshida et al. 1983b; selected, Mackay et al. 1985)

$k_{OH} = (8.8 \pm 1) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with estimated atmospheric lifetime $\tau = 13$ d and $k_{O3} < 5 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} with lifetime $\tau > 8.8$ yr at room temp. (relative rate method, Atkinson et al. 1985)

k_{OH} (obs.) = 9.4×10^{-13} cm^3 molecule^{-1} s^{-1}; and k_{OH}(calc) = 1.6×10^{-13} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1985)

$k_{OH} = (5.5 \pm 4.4) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 23.5°C with an atmospheric lifetime $\tau = 21$ d (relative rate method, Edney et al. 1986)

$k_{OH} = 9.4 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} with $t_{1/2} = 17$ d for reaction with OH radical, concn of 5.0×10^5 molecule/cm^3 at room temp. (Atkinson 1987)

k_{OH}(calc) = 1.4×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs) = 0.71×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH}* = $(7.41 \pm 0.94) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{OH} = 7.41 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}; k(soln) = 9.1×10^{-12} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k = (4.3–4.6) \times 10^9$ M^{-1} s^{-1} for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{OH} = 7.7 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH}(calc) = 0.70×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982);

base rate constant $k < 0.9$ M^{-1} h^{-1} with $t_{1/2} > 900$ yr, based on assumed base mediated 1% disappearance after 16 d at 85°C and pH 9.7 (Ellington et al. 1988).

$t_{1/2} > 879$ yr based on rate constant $k < 0.9$ M^{-1} h^{-1} extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Ellington et al. 1988)

Biodegradation: significant degradation on anaerobic environment with $k = 0.5$ d^{-1} (Tabak et al. 1981; Mills et al. 1982)

$k = 1.88 \times 10^{-4}$ h^{-1} in air, and $k = 3.83 \times 10^{-4}$ h^{-1} in sediments (Lee & Ryan 1979; selected, Mackay et al. 1985)

$k = 0.24$ L d^{-1} in air, no degradation in water and on the ground (Neely 1982);

$k = 0.07–0.3$ d^{-1} in river water; $k = 0.04–0.2$ d^{-1} in estuary water; and $k = 0.01$ d^{-1} in marine water (Bartholomew & Pfaender 1983; selected, Battersby 1990)

$k = 0.033$ d^{-1}, $t_{1/2} = 21$ d in spring at 8–16°C, $k = 0.152$ d^{-1}, $t_{1/2} = 4.6$ d in summer at 20–22°C, $k = 0.053$ d^{-1}, $t_{1/2} = 13$ d in winter at 3–7°C, and $k = 0.08$ d^{-1}, $t_{1/2} = 8.9$ d with $HgCl_2$ in September 9–15, 1980 in marine mesocosm system (Wakeham et al. 1983)

$t_{1/2} = 4.6–21$ d in marine mesocosm (Wakeham et al. 1983);

$t_{1/2} = 7.9$ d in activated sludge (estimated, Freitag et al. 1985, quoted, Anderson et al. 1991);

$k = 0.07$ yr^{-1} with $t_{1/2} = 37$ d (Olsen & Davis 1990)

$t_{1/2}$(aq. aerobic) = 1632–3600 h, based on unacclimated aerobic river dieaway tests; $t_{1/2}$(aq. anaerobic) = 6528–14400 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation: 3×10^{-9} mL cell^{-1} h^{-1} (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1), and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photodecomposition $t_{1/2} = 8.7$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976);

residence time of 13 d, loss of 7.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

estimated atmospheric lifetime $\tau = 13$ d due to reaction with OH radical and $\tau > 8.8$ yr due to reaction with O_3 (Atkinson et al. 1985);

$t_{1/2} = 72.9–729$ h, based on photooxidation half-life in air (Howard et al. 1991).

Surface Water: $t_{1/2} = 0.3$ d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 75$ d for an estuarine river with near natural conditions at 22°C (Lee & Ryan 1976);

rate constants: $k = 0.033$ d^{-1}, $t_{1/2} = 21$ d in spring at 8–16°C, $k = 0.152$ d^{-1}, $t_{1/2} = 4.6$ d in summer at 20–22°C, $k = 0.053$ d^{-1}, $t_{1/2} = 13$ d in winter at 3–7°C for periods when volatilization appears to dominate, and $k = 0.08$ d^{-1}, $t_{1/2} = 8.9$ d with $HgCl_2$ in September 9–15, 1980 in marine mesocosm experiments (Wakeham et al. 1983)

$t_{1/2}$ = 1632–3600 h, based on unacclimated aerobic river dieaway tests (Howard et al. 1991)
photolysis $t_{1/2}$ = 21 d under sunlight in water (Mansour & Feicht 1994).
Groundwater: $t_{1/2}$ = 3264–7200 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: $t_{1/2}$ = 75 d (Lee & Ryan 1976, 1979; quoted, Anderson et al. 1991).
Soil: disappearance $t_{1/2}$ = 2.1 d from testing soils (Anderson et al. 1991);
$t_{1/2}$ = 1632–3600 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biota:

TABLE 6.1.1.1.1
Reported aqueous solubilities of chlorobenzene at various temperatures

1.

Kisarov 1962		**Nelson & Smit 1978**		**Schwarz & Miller 1980**		**Horvath & Getzen 1985**	
shake flask		**vapor equil.-UV spec.**		**elution chromatography**		**recommended values**	
t/°C	**S/g·m⁻³**	**t/°C**	**S/g·m⁻³**	**t/°C**	**S/g·m⁻³**	**t/°C**	**S/g·m⁻³**
30	490	5	40	10	440	10	454
40	705	25	106.8	20	420	15	452
50	960	35	400.5	30	490	20	466
60	1100	45	471.3	shake flask UV		25	495
70	1605			10	460	30	539
80	1805			20	450	35	600
90	2500			30	500	40	677
						45	771
						50	882
						55	1011
						60	1158
						65	1324
						70	1509
						75	1713
						80	1937
						90	2447

2.

Cooling et al. 1992		**Ma et al. 2001**		**Finizio & Di Guardo 2001**	
shake flask-GC/MS		**shake flask-GC**		**RP-HPLC-k′ correlation**	
t/°C	**S/g·m⁻³**	**t/°C**	**S/g·m⁻³**	**t/°C**	**S/g·m⁻³**
20	482	5	496	5	426
30	608	15	429	15	427
40	840	25	470	35	511
50	1263	35	538		
		45	546		

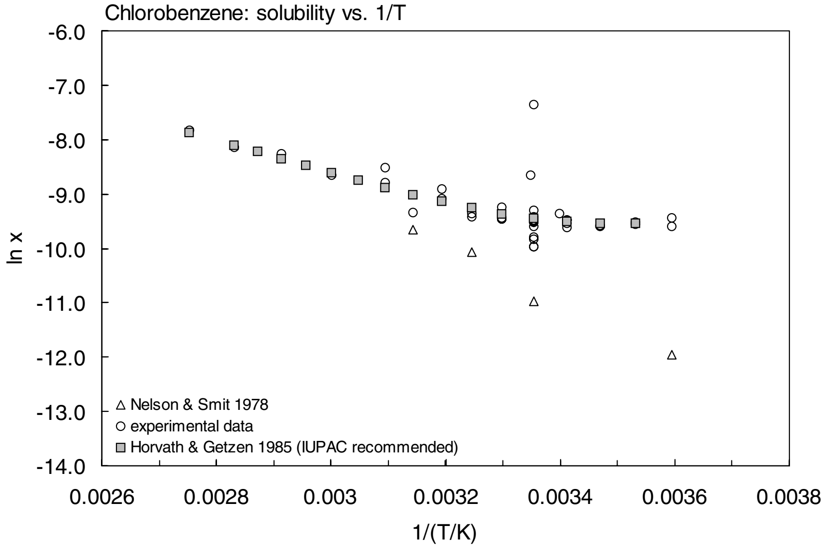


FIGURE 6.1.1.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.2
Reported vapor pressures of chlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		Dreisbach & Shrader 1949		Brown 1952		Liu & Dickhut 1994	
summary of lit. data		ebulliometry		ebulliometry		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–13.0	133.3	56.28	7605	62.04	9657	–14.2	66.9
10.6	666.6	63.05	10114	62.06	9663	–5.0	167
22.2	1333	75.22	16500	66.38	11558	10	501
35.3	2666	101.85	42066	74.13	15720	25	1410
49.7	5333	117.30	67661	89.06	27246	40	3270
58.3	7999	131.70	101325	94.04	32276		
70.0	13332			98.79	37961		
89.4	26664			110.35	54794	ΔH_V = 35.6 kJ/mol	
110	53329	mp/°C	–45.58	121.1	69774		
132.2	101325	bp/°C	131.67	126.18	87018	ΔH_{subl} = 35.6 kJ/mol	
				130.37	97684		
mp/°C	–45.2	eq. 2	P/mmHg	131.7	101263		
		A	7.18473				
		B	1556.6	eq. 2	P/mmHg		
		C	230	A	6.99893		
				B	1444.75		
				C	219.13		

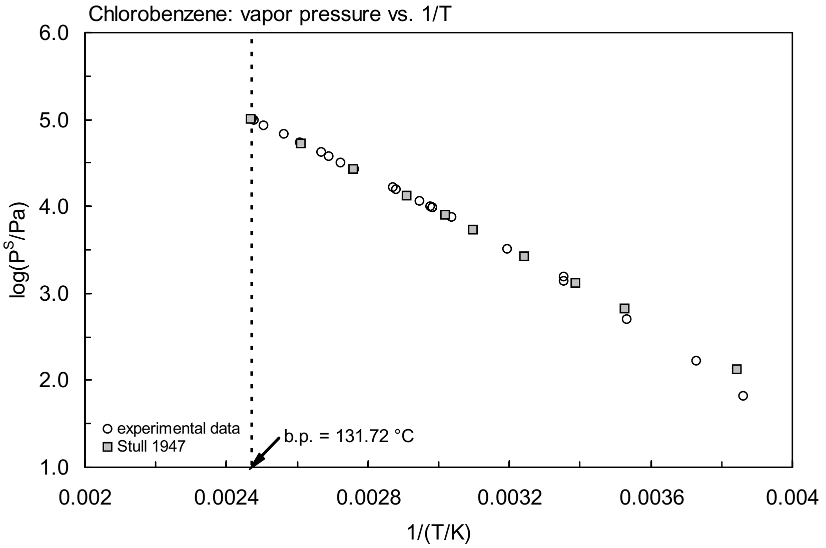


FIGURE 6.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.3
Reported Henry's law constants of chlorobenzene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln k_H = A - B/(T/K)$	(3)	$\log k_H = A - B/(T/K)$	(3a)
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

1.

Leighton & Calo 1981		Ashworth et al. 1988		Ettre et al. 1993		Görgényi et al. 2002	
equilibrium cell-concn ratio		EPICS-GC		equilibrium headspace-GC		EPICS-SPME method	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1	124	10	247	45	621	2	112
3	125	15	285	60	863	6	155.5
12.4	190	20	346	70	1114	10	183.6
12.5	206	25	365	80	1579	18	283.2
17.9	243	30	479			25	384
19.1	280					30	472.8
22.7	271	eq. 4	H/(atm m³/mol)	eq. 2a	$1/K_{AW}$	40	755.8
23	321	A	3.469	A	2.905024	50	1046
		B	2689	B	1129.8083	60	1420
eq. 3	k_H/atm					70	1804
A	18.46						
B	3751					eq. 1	K_{AW}
						A	10.04
						B	3359.7

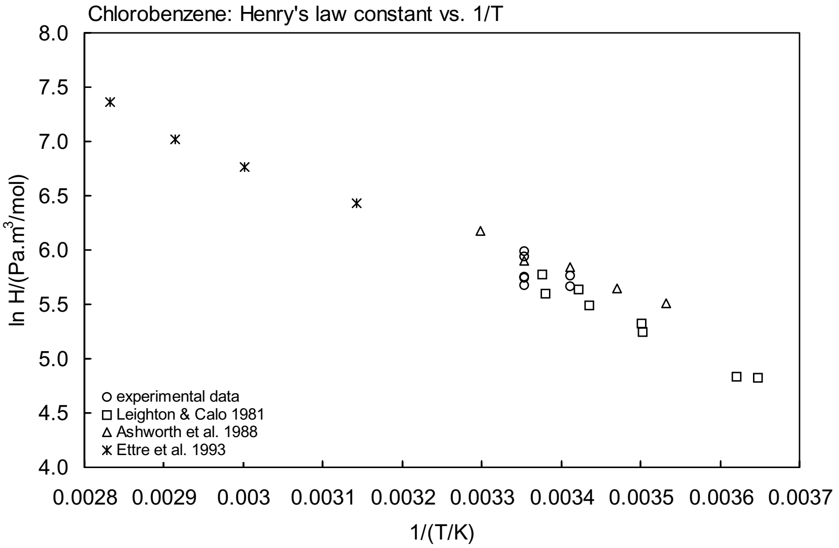


FIGURE 6.1.1.1.3 Logarithm of Henry's law constant versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.4
Reported octanol-water and octanol-air partition coefficients of chlorobenzene at various temperatures

log K_{OW}		log K_{OA}	
Finizio & Di Guardo 2001		Su et al. 2002	
GC-RT correlation		GC-RT correlation	
t/°C	log K_{OW}	t/°C	log K_{OA}
5	3.19	10	3.76
15	3.15	20	3.45
25	3.05	30	3.17
35	3.04	40	2.90
		50	2.65
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 43.91$	
		log K_{OA} = A + B/T	
		A	– 4.107
		B	43910

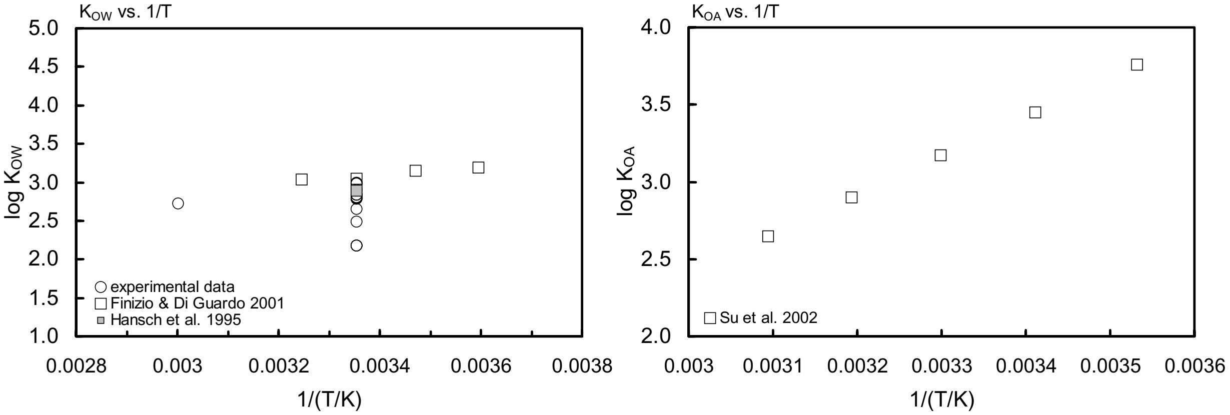
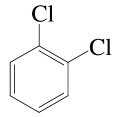


FIGURE 6.1.1.1.4 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for chlorobenzene.

6.1.1.2 1,2-Dichlorobenzene



Common Name: 1,2-Dichlorobenzene
Synonym: *o*-dichlorobenzene, dowtherm E
Chemical Name: 1,2-dichlorobenzene
CAS Registry No: 95-50-1
Molecular Formula: $C_6H_4Cl_2$
Molecular Weight: 147.002
Melting Point (°C):
  –17.0 (Pirsch 1956; Dreisbach 1955; Weast 1972–73; 1982–83; Lide 2003)
Boiling Point (°C):
  180 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.3048 (Weast 1972–73; Horvath 1982)
  1.3059 (Lide 2003)
Molar Volume (cm^3/mol):
  112.6 (20°C, calculated-density)
  137.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  12.93 (Weast 1972–73)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  50.46 (Pirsch 1956)
  50.63 (Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  145* (volumetric, measured range 20–60°C, Klemenc & Low 1930; Seidell 1941)
  < 260 (residue-volume method, Booth & Everson 1948)
  92.7 (Landolt-Börnstein 1951)
  79.0 (shake flask-radiolabeled ^{14}C-LSC, Metcalf et al. 1975)
  148* (20°C, shake flask-GC/ECD, measured 0–34°C, Chiou & Freed 1977)
  92.8 (shake flask-UV, Yalkowsky et al. 1979)
  154 (shake flask-LSC/^{14}C, Veith et al. 1980)
  128, 124* (20°C; elution chromatography, UV, Schwarz & Miller 1980)
  155.8 (shake flask-LSC, Banerjee et al. 1980; Banerjee 1985)
  99.1 (shake flask-GC, Könemann 1981)
  92.6 (recommended, Horvath 1982)
  154 (shake flask-GC, Chiou et al. 1982, 1983; Chiou 1981, 1985; Chiou & Schmedding 1981)
  125 (quoted average, Yalkowsky et al. 1983)
  92.3 (generator column-GC, Miller et al. 1984, 1985)
  137 (shake flask-HPLC, Banerjee 1984)
  147* (recommended, temp range 0–60°C, IUPAC Solubility Data Series, Hovath & Getzen 1985)
  $S/(g/kg) = 19.2314 - 1.81140 \times 10^{-1}\cdot(T/K) + 5.6509 \times 10^{-4}\cdot(T/K)^2 - 5.77683 \times 10^{-7}\cdot(T/K)^3$, temp range 273–333 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)
  169 (shake flask-radiometry, Lo et al. 1986)
  156 (quoted lit. average, Riddick et al. 1986; Howard 1989)
  31* (19.5°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1992)
  145 (dialysis tubing equilibration-GC. Etzweiler et al. 1995)

159.2 (shake flask-GC/ECD, Tam et al. 1996)
144 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
109 (shake flask-GC, Boyd et al., 1998)
92, 93, 137; 97 (quoted lit. values; solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
$\ln x = -31.5289 + 3834/(T/K) + 8.7172 \times 10^{-5} \cdot (T/K)^2$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
149* ± 8.2 (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)
140, 124, 158 (5, 15, 25°C, estimated-RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)
93.7* (generator column-GC/ECD, measured range 15–55°C, Oleszek-Kudlak et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

137* (20°C, summary of literature data, Stull 1947)
$\log (P/mmHg) = 7.32585 - 1824.6/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
5010* (56.28°C, ebulliometry, measured range 87.02–180.48°C, Dreisbach & Shrader 1949)
171 (calculated by formula., Dreisbach 1955)
$\log (P/mmHg) = 6.92400 - 1538.3/(200.0 + t/°C)$; temp range 80–250°C (Antoine eq. for liquid state, Dreisbach 1955)
25234* (130.82°C, ebulliometry, measured range 130.82–181.62°C, McDonald et al. 1959)
196 (extrapolated, Antoine eq., Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 10943.0/(T/K)] + 8.185275$; temp range 20–179°C (Antoine eq., Weast 1972–73)
174, 197 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
224.87*; 132, 188 (27.8°C reported; 20°C, 25°C, extrapolated-Antoine eq. from gas saturation-GC measurement, temp range 27.8–70°C, Grayson & Fosbraey 1982)
$\log (P/Pa) = 25.4 - 6013/(T/K)$, temp range 27.8–70°C (gas saturation-GC, Grayson & Fosbraey 1982)
$\log (P/kPa) = 6.13305 - 1599.034/(206.964 + t/°C)$; temp range 87.2–180.5°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
$\log (P/kPa) = 6.26861 - 1704.435/(219.409 + t/°C)$; temp range 130.8–181.62°C (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1984)
197 (extrapolated, Antoine eq., Dean 1985)
$\log (P/mmHg) = 7.14378 - 1704.49/(219.42 + t/°C)$; temp range 131–181°C (Antoine eq., Dean 1985, 1992)
201.4 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
198 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.26918 - 1705.55/(-52.56 + T/K)$; temp range 373–453 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
164* (gas saturation, measured range –15 to 40°C, Liu & Dickhut 1994)
137.3*; 188 (pressure gauge measured at 20.35°C, 25°C, interpolated from reported Antoine eq., Polednicek et al. 1996)
$\ln (P/Pa) = 21.5929 - 4053.86/[(T/K) - 50.2328]$; temp range 256–422 K (Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
252; 185 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
$\log (P/mmHg) = 31.3614 - 3.5226 \times 10^3/(T/K) - 7.8886 \cdot \log (T/K) - 2.2250 \times 10^{-10} \cdot (T/K) + 1.1842 \times 10^{-6} \cdot (T/K)^2$, temp range 256–705 K (Yaws 1994)
5729* (90.193°C, comparative ebulliometry, measured range 90.193–181.633°C, Roháč et al. 1998)
133.8* (20°C, recommended, summary of literature data, temp range 263.15–463.15 K, Roháč et al. 1999)
$\ln [(P/Pa)/6.80] = [1 - (T/K)/256.10] \cdot \exp\{3.359374 - 8.5641422 \times 10^{-4} \cdot (T/K) + 6.0235167 \times 10^{-7} (T/K)^2\}$; temp range 256–445 K (Cox eq., recommended, Roháč et al. 1999)
$\log (P/kPa) = 19.40 - 6013/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

248 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
375 (calculated-bond contribution, Hine & Mookerjee 1975)
193 (batch air stripping-GC, Mackay & Shiu 1981)
122 (20°C, gas stripping-GC, Oliver 1985)

197 (gas stripping, Warner et al. 1987)
159* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln $[H/(atm{\cdot}m^3/mol)] = -1.518 - 1422/(T/K)$; temp range 10–30°C (EPICS-GC/FID, Ashworth et al. 1988)
299 (computer value, Yaws et al. 1991)
141 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
195 (gas stripping-GC, Shiu & Mackay 1997)
212.7 (modified EPICS method-GC, Ryu & Park 1999)
133 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 7.045 - 2636/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

3.55 (Hansch et al. 1968)
3.38 (Leo et al. 1971; Hansch & Leo 1979, 1985)
3.57 (calculated-fragment constants, Rekker 1977)
3.55, 3.39 (shake flask-GC, HPLC-k′, Könemann et al. 1979)
3.40; 3.75 (concentration ratio; HPLC-RT correlation, Veith et al. 1980)
3.40 (shake flask-LSC, Banerjee et al. 1980)
3.71, 3.18–4.36 (shake flask method: mean, range of mean values, OECD 1981)
3.34 (shake flask-HPLC, Hammers et al. 1982)
3.40 (shake flask-GC, Watarai et al. 1982)
3.19, 3.19, 3.31, 3.53, 3.60, 3.84, 4.15, 4.36; 3.61 (shake flask; results of OECD/EEC laboratory comparison tests; mean value, Harnisch et al. 1983)
3.34, 3.20; 3.61 (HPLC methods; OECD/EEC shake-flask method; Harnisch et al. 1983)
3.61 (OECD/EEC shake-flask method, Harnisch et al. 1983)
3.38 (generator column-HPLC/UV, Wasik et al. 1983)
3.38 (generator column-GC, Miller et al. 1984, 1985)
3.56 (HPLC-RV correlation, Garst 1984)
3.433 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
3.49 (shake flask-GC, Pereira et al. 1988)
3.38 (recommended, Sangster 1993)
3.43 (recommended, Hansch et al. 1995)
3.29 ± 0.05 (shake flask-GC/ECD, Bahadur et al. 1997)
3.29* (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)
$\log K_{OW} = 0.1831 + 17800/[2.303{\cdot}R(T/K)]$; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
3.447 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
3.70 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrăder 1999)

Octanol/Air Partition Coefficient, log K_{OA} and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

4.36*, 4.41 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
$\log K_{OA} = -4.30 + 2574.0/(T/K)$; $\Delta H_{OA} = 49.3$ kJ/mol (generator column-GC, Harner & Mackay 1995)
4.68 (solid-phase microextraction SPME-GC, Treves et al. 2001)
$\log K_{OA} = -7.90 + 3304/(T/K)$, $\Delta H_{OA} = 63.3$ kJ/mol (SPME-GC, Treves et al. 2001)

Bioconcentration Factor, log BCF at 25°C or as indicated:

1.95 (bluegill sunfish, Veith et al. 1979b; 1980)
2.19–2.48 (fish, calculated, Veith et al. 1980)
1.95 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
2.86 (microorganisms-water, Mabey et al. 1982)
2.40–2.48 mean 2.43; 2.60–2.85 mean 2.74 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
3.51–3.80 (rainbow trout, lipid-basis, Oliver & Niimi 1983)
2.43–2.75 (fish, Oliver 1984)
1.95 (correlated-flow through method, bluegill sunfish, Davis & Dobbs 1984)

1.60 (fish-normalized, Tadokoro & Tomita 1987)

1.89 (fish, calculated-MCI χ, Sabljic 1987b)

3.94, 4.46, 3.79, 3.82 (field data: Atlantic croaker, blue crabs, spotted sea trout, blue catfish, lipid-based, Pereira et al. 1988)

2.4 ± 0.1 (guppies, steady-state conditions, rate const. ratio k_1/k_2, 96-h exposure, Sijm et al. 1993)

3.5 ± 0.1 (guppies, lipid normalized BCF, Sijm et al. 1993)

2.70 (fathead minnow, steady-state conditions, rate const. ratio k_1/k_2, 96-h exposure, Sijm et al. 1993)

3.90 (fathead minnow, lipid normalized BCF, Sijm et al. 1993)

1.95; 2.43, 2.75 (*Lepomis macrochirus; Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)

2.40; 2.70 (*Poecilla reticulata; Pimephales promelas*, quoted lit., static and semi-static conditions, Devillers et al. 1996)

2.43, 3.51; 2.333, 2.549 (quoted: whole fish, lipid content; calculated-MCI χ, calculated-K_{OW}, Lu et al. 1999)

3.86; 3.84 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

2.26 (Willamette silt loam soil, 1.6% organic matter, equilibrium sorption isotherm measurement, Chiou et al. 1979)

3.0, 2.96, 2.62 (calculated-K_{OW}, solubility C_L, C_S, Karickhoff 1981)

4.60; 4.60; 3.00 (field data of sediment trap material, Niagara River organic matter, calculated from K_{OW}, Oliver & Charlton 1984)

2.34, 2.59 (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)

2.45 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

3.27, 2.04 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

2.43 (untreated Marlette soil B_t horizon, OC 0.30%, batch equilibrium, Lee et al. 1989)

3.64, 3.52 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

2.45–3.51 (aquifer materials, Stauffer et al. 1989)

3.10, 2.90; 2.99 (Captina silt loam, OC 1.49% and pH 4.97, McLaurin sandy loam, OC 0.66%, pH 4.43; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

2.36–2.61 (16 U.S. soils, 1.03–6.09% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)

2.37–2.51 (16 Chinese soils, 0.16–5.61% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)

2.48–2.76 (14 U.S. bed sediments, 0.4–2.20% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)

2.62–2.78 (21 Chinese bed sediments, 0.11–4.73% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)

2.36–2.63 (suspended solids from four U.S. rivers, 1.78–2.87% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)

2.48 (suspended solids from Yellow River, China, 0.30% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)

2.39, 2.40 (RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

3.69 ± 0.74 (suspended particulate in coastal waters, Masunaga et al. 1996)

2.50, 2.50, 2.47 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, 0.1 $\leq$ OC < 0.5%, average, Delle Site 2001)

2.70, 2.69, 2.71 (sediments, organic carbon OC $\leq$ 0.1%, OC $\leq$ 0.5%, 0.1 $\leq$ OC < 0.5%, average, Delle Site 2001)

Sorption Coefficient, log K_{OM}:

2.25 (Willamette silt loam soil, 1.6% organic matter, equilibrium isotherm, Chiou et al. 1979; quoted, Howard 1989)

2.27 (Woodburn silt loam soil, 1.9% organic matter, batch equilibrium-sorption isotherm-GC/ECD, Chiou et al. 1983)

2.50 (soil, Chiou et al. 1983)

2.26, 2.54 (quoted, calculated-MCI χ, Sabljic 1984)

2.89 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.47, 3.17 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.97 (untreated Marlette soil B_t horizon, OM 0.60%, equilibrium isotherm, Lee et al. 1989)
3.97, 3.50, 2.87 (organic cations treated Marlette soil B_t horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization/Evaporation: experimental evaporation rate into air, 1.18×10^{-6} g cm^{-2} s^{-1} (Chiou et al. 1980); estimated $t_{½}$ = 4.4 h for a model river of 1-m depth with a flow rate of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: not environmentally significant (Mabey et al. 1982); rate constant k = 1.22×10^{-4} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical, and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} ~ 3.0×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

k << 360 M^{-1} h^{-1} for singlet oxygen and << 1 M^{-1} h^{-1} for RO_2 radical (Mabey et al. 1982)

k_{OH} = $(4.2 \pm 0.2) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

k_{O3} = 2.0×10^{-23} cm^3 $molecule^{-1}$ s^{-1} at 298 K measured range 298–323 K (Atkinson & Carter 1984)

k_{OH} (obs.) = 4.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1}; and k_{OH}(calc) = 4.9×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1985)

k_{OH}(calc) = 4.1×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs) = 4.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH} = 4.07×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 22–27°C (Dilling et al. 1988)

k = (3.7–4.0) × 10^{-9} M^{-1} s^{-1} for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

k_{OH}(calc) = 4.0×10^{9} M^{-1} s^{-1} in aqueous solutions (Haag & Yao 1992)

k_{OH}(calc) = 0.48×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982).

base rate constant k < 0.9 M^{-1} h^{-1} at 25°C with a calculated $t_{½}$ > 900 yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

Biodegradation: $t_{½}$(aq. aerobic) = 672–4320 h, based on unacclimated soil grab sample data, and aerobic screening test data (Howard et al. 1991);

$t_{½}$(aq. anaerobic) = 2880–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

significant degradation in an aerobic environment with k = 0.05 d^{-1} (Tabak et al. 1981; Mills et al. 1982); in a continuous flow of activated sludge system; virtually 100% (78% biodegradation and 22% stripping) was observed (Kincannon et al. 1983; selected, Howard 1989).

Biotransformation: 1×10^{-10} ml $cell^{-1}$ h^{-1} (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1), and Elimination (k_2) Rate Constants:

k_1 = 870 L kg^{-1} d^{-1}; k_2 = 3.90 d^{-1} (guppy, 96-h exposure., Sijm et al. 1993)

k_1 = 635 L kg^{-1} d^{-1}; k_2 = 1.40 d^{-1} (fathead minnow, 96-h exposure, Sijm et al. 1993)

Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{½}$ = 152.8–1528 h, based on the photooxidation half-life in air. (Howard et al. 1991)

Surface water: $t_{½}$ = 1.2–37 d estimated from field data at various locations in the Netherlands, $t_{½}$ = 0.3–3 d for river, $t_{½}$ = 3–30 d for lakes (Zoeteman et al. 1980)

$t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Groundwater: $t_{½}$ = 30–300 d, estimated from persistence in water (Zoeteman et al. 1980);

$t_{1/2}$ ~1 yr estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)
$t_{1/2}$ = 1344–8640 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Sediment:
Soil: $t_{1/2}$ = 672–4320 h, based on unacclimated aerobic screening test data (Howard et al. 1991)
disappearance $t_{1/2}$ = 4.0 d in testing soils (Anderson et al. 1991).
Biota: $t_{1/2}$ < 1 d in fish (Veith et al. 1980);
$t_{1/2}$ < 1 d bluegill sunfish. (Barrows et al. 1980);
$t_{1/2}$ < 5 d in worms at 8°C (Oliver 1987a);
biological half-lives: $t_{1/2}$ < 1 d in trout muscle, $t_{1/2}$ < 1 d in sunfish and $t_{1/2}$ < 1 d in guppy for dichlorobenzenes (Niimi 1987).

TABLE 6.1.1.2.1
Reported aqueous solubilities of 1,2-dichlorobenzene at various temperatures

1.

Klemenc & Löw 1930		Chiou & Freed 1977		Schwarz & Miller 1980		Horvath & Getzen 1985	
volumetric method		shake flask-GC		elution chromatography		recommended values	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
20	134	0	133	10	169	0	142
25	145	20	148	20	128	5	135
30	161	34	162	shake flask-UV		10	133
35	183			10	156	15	134
40	194			20	124	20	139
45	203					25	147
55	223					30	157
60	232					35	169
						40	182
						45	197
						50	212
						55	228
						60	243

2.

Stephenson 1992		Ma et al. 2001		Finizio & Di Guardo 2001		Oleszek-Kudlak et al. 2004	
shake flask-GC		shake flask-GC/FID		RP-HPLC-k′ correlation		generator column-GC/ECD	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
0	50	5	127	5	140	25	93.7
19.5	31	15	132	15	124	25	94.4
40	17	25	149	35	158	35	108.0
50	24	35	162			45	122.7
60.5	54	45	204			55	130.1
70.7	55						
80.0	91					ΔH_{sol} = 10.49 kJ/mol	
90.5	83						

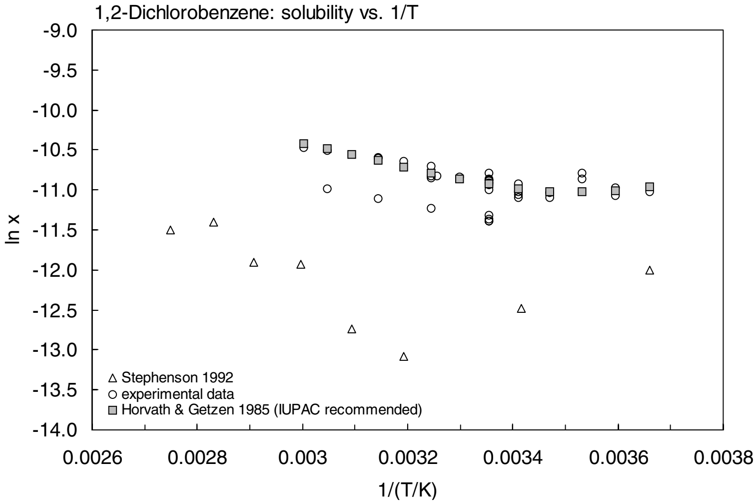


FIGURE 6.1.1.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,2-dichlorobenzene.

TABLE 6.1.1.2.2
Reported vapor pressures of 1,2-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln (P/Pa) = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_o) = (1 - T/T_o) \cdot \exp[\Sigma A_i T^i]$	(5) - Cox eq.		

1.

Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959		Grayson & Fosbraey 1982	
summary of lit. data		ebulliometry		ebulliometry		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	133.3	87.02	5010	130.82	25234	20.0	132
46	666.6	97.66	7605	154.83	51778	27.8	224.8
59.1	1333	104.94	10114	178.66	96998	32.0	282.8
73.4	2666	118.32	16500	179.73	99614	41.5	599.3
89.4	5333	147.6	42066	180.54	101655	48.6	780.1
99.5	7999	164.65	67661	181.62	104322	56.3	1253
112.9	13332	180.48	101325			61.1	1645
133.4	26664			mp/°C	–17.0	70.0	2636
155.8	53329						
180	101325	eq. 2	P/mmHg	eq. 2	P/mmHg		
		A	7.32585	A	7.07028	eq. 1	P/Pa
mp/°C	–17.6	B	1824.6	B	1649.55	A	25.4
		C	230	C	213.314	B	6013

TABLE 6.1.1.2.2 (*Continued*)

2.

Liu & Dickhut 1994		Polednicek et al. 1996		Roháč et al. 1998		Roháč et al. 1999	
gas saturation-GC		pressure gauge		comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–14.2	7.73	–16.65	7.056	90.193	5729	263.15	12.9
–5.0	14.7	–16.65	7.042	99.529	8333	273.15	30.1
10	56.1	–9.75	13.175	99.53	8335	283.15	65.4
25	164	–9.75	13.195	107.0	11074	283.15	133.8
40	448	0.30	30.815	113.265	13917	303.15	259.1
		10.32	67.088	118.61	16800	313.15	477.9
		20.35	137.3	118.61	16799	232.15	843.3
$\Delta H_V/(\text{kJ mol}^{-1}) = 51.2$		30.28	264.39	124.14	20290	333.15	1430
		40.24	485.45	129.935	24569	343.25	2338
exptl data fitted to the		50.15	848.67	135.547	29394	353.15	3699
modified Watson correlation		60.15	1440.7	141.024	34818	363.15	5681
		60.15	1442.0	146.292	40757	373.15	8491
		70.05	2313.0	146.292	40761	383.15	12380
		70.05	2318.6	151.657	47825	393.15	17640
		80.02	3660.3	160.102	60273	403.15	24630
		80.03	3661.2	168.184	74765	413.15	33720
		88.75	5428.4	176.912	93403	423.15	45370
		88.75	54284	178.845	97970	433.15	60070
		89.94	5606.9	181.633	104893	443.15	78370
		89.94	5601.2			453.15	10080
		98.79	8102.5	bp/°C	180.190	463.15	12810
		98.79	8104.0				
		108.76	11826	eq. 3	P/kPa	Cox eq.	
		118.8	16870	A	6.16161	eq. 5	
		128.19	23583	B	1612.27	A_0	3.359374
		138.83	32396	C	–64.447	$10^{-4}A_1$	–8.5641422
		148.91	43690			$10^{-7}A_2$	6.0235167
						T_o/K	256.10
		eq. 3a	P/Pa			P_o/Pa	6.80
		A	21.5929			bp/K	453.35
		B	4053.86			temp range 256–445 K	
		C	–50.2358				

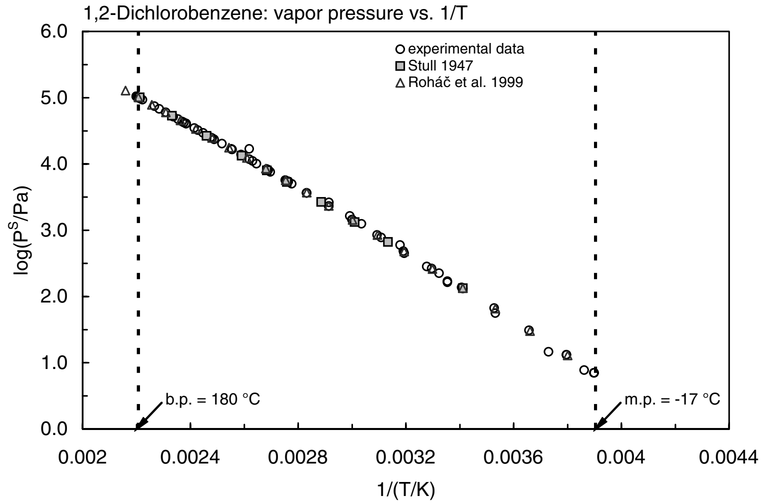


FIGURE 6.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichlorobenzene.

TABLE 6.1.1.2.3
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,2-dichlorobenzene at various temperatures and temperature dependence equations

Henry's law constant		log K_{OW}		log K_{OA}			
Ashworth et al. 1988		Bahadur et al. 1997		Harner & Mackay 1995		Su et al. 2002	
EPICS		shake flask-GC/ECD		generator column-GC		GC-RT correlation	
t/°C	H/(Pa m^3/mol)	t/°C	log K_{OW}	t/°C	log K_{OA}	t/°C	log K_{OA}
10	165	5	3.51	–10	5.51	10	4.6
15	145	15	3.41	0	5.16	20	4.27
20	170	25	3.29	10	4.82	30	3.96
20	159	35	3.2	20	4.51	40	3.67
30	240	45	3.09			50	3.4
		enthalpy of transfer		ΔH_{OA}/(kJ mol^{-1}) = 49.3		ΔH_{OA}/(kJ mol^{-1}) = 57.02	
ln H = A – B/(T/K)		ΔH/(kJ mol^{-1}) = –17.8		.			
	H/(atm m^3/mol)			log K_{OA} = A + B/RT		log K_{OA} = A + B/2.303RT	
A	–1.518	log K_{OW} = A – ΔH/2.303RT		A	–4.3	A	–5.856
B	1422	A	0.1831	B	2574	B	57020
		ΔH	–17800				

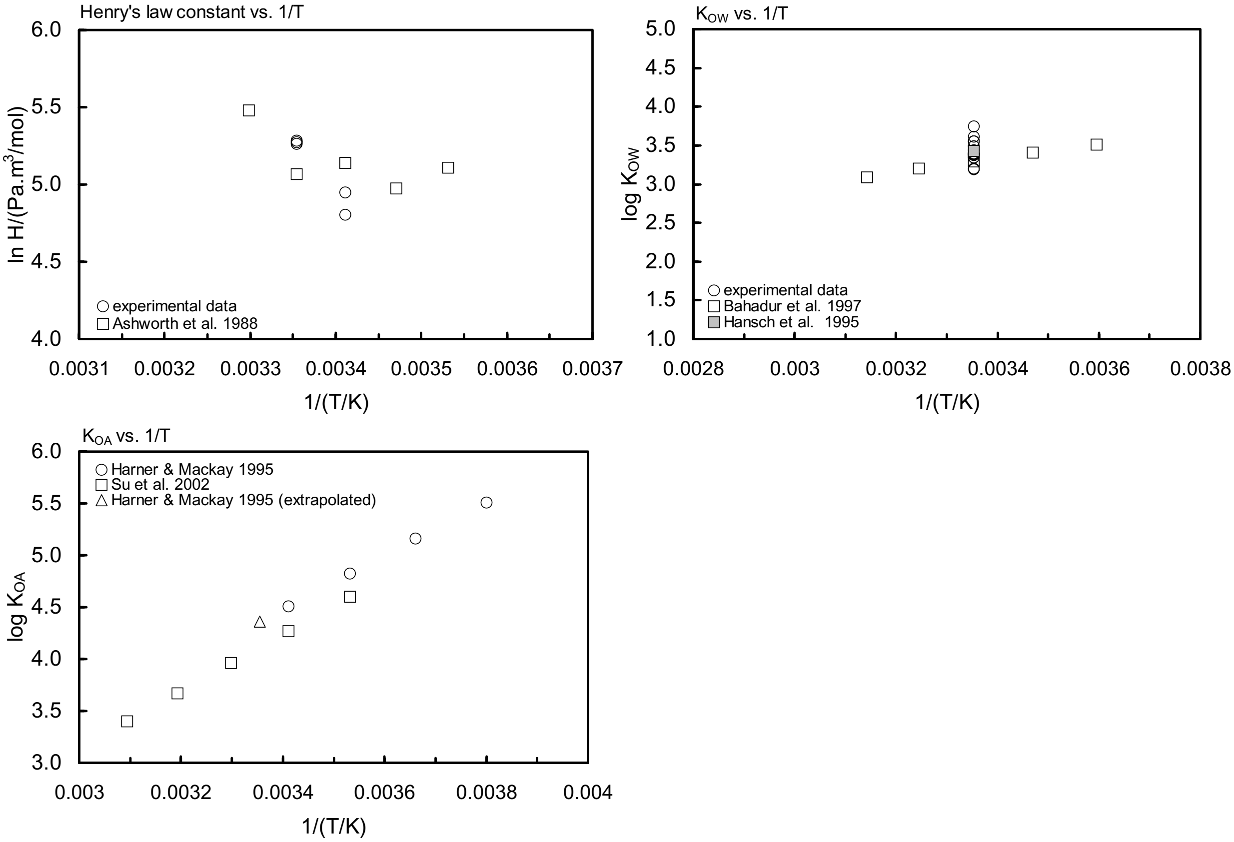
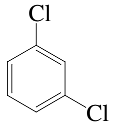


FIGURE 6.1.1.2.3 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for 1,2-dichlorobenzene.

6.1.1.3 1,3-Dichlorobenzene



Common Name: 1,3-Dichlorobenzene
Synonym: *m*-dichlorobenzene
Chemical Name: 1,3-dichlorobenzene
CAS Registry No: 541-73-1
Molecular Formula: $C_6H_4Cl_2$
Molecular Weight: 147.002
Melting Point (°C):
–24.8 (Lide 2003)
Boiling Point (°C):
173 (Lide 2003)
Density (g/cm^3 at 20°C):
1.2884 (Dreisbach 1955; Weast 1972–73; Horvath 1982; Lide 2003)
Molar Volume (cm^3/mol):
114.1 (20°C, calculated-density)
137.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
12.64 (Weast 1972–73)
Entropy of Fusion, ΔS_{fus} (J/mol K):
50.63 (Pirsch 1956)
51.46 (Yalkowsky 1979)
51.05 (Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
123* (volumetric, measured range 20–60°C, Klemenc & Löw 1930)
123.5 (Ginnings et al. 1939)
124 (Landolt-Börnstein 1951)
101.26* (shake flask-UV, measured range 10–35°C, Vesala 1973)
102.9 (shake flask-UV, Vesala 1974)
119.5 (shake flask-UV, Yalkowsky et al. 1979)
131 (shake flask-LSC-^{14}C, Veith et al. 1980)
144*, 149 (23.5°C, elution chromatography, measured range 10–30°C, Schwarz 1980)
111, 89, 113, 101 (20°C, quoted, UV, elution chromatography, average exptl. value, Schwarz & Miller 1980)
133.5 (shake flask-LSC, Banerjee et al. 1980)
68.6 (shake flask-GC, Könemann 1981)
134 (shake flask-GC/ECD, Chiou & Schmedding 1981; Chiou et al. 1982, 1983; Chiou 1985)
124 (recommended, Horvath 1982)
124.5 (generator column-GC/ECD, Miller et al. 1984, 1985)
143 (shake flask-HPLC, Banerjee 1984)
106* (recommended, temp range 10–60°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)
$S/(g/kg) = 27.6827 - 2.61597 \times 10^{-1} \cdot (T/K) + 8.19706 \times 10^{-4} \cdot (T/K)^2 - 8.4698 \times 10^{-7} \cdot (T/K)^3$, temp range 283–333 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)
110 (Dean 1985)
111 (20°C, Riddick et al. 1986)
130 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
123; 138 (quoted lit.; shake flask-GC, Boyd et al. 1998)

126* ± 6.1 (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)
71, 104, 132, 166 (5, 15, 25, 35°C, estimated-RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (12.1°C, summary of literature data, Stull 1947)
log (P/mmHg) = 7.30364 – 1782.4/(C + t/°C) (Antoine eq., Dreisbach & Martin 1949)
7605* (90.72°C, ebulliometry, measured range 90.72–173.0°C, Dreisbach & Shrader 1949)
252 (calculated by formula., Dreisbach 1955)
log (P/mmHg) = 6.88045 – 1496.2/(201.0 + t/°C); temp range 75–240°C (Antoine eq. for liquid state, Dreisbach 1955)
307 (extrapolated, Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 10446.8/(T/K)] + 8.017555; temp range 12.1–173°C (Antoine eq., Weast 1972–73)
266 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.17083 – 1611.121/(213.817 + t/°C); temp range 90.7–173°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
179.3 (gas saturation, interpolated from reported graph, Rordorf 1985)
265 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.0401 – 1607.05/(213.38 + t/°C); temp range 91–173°C (Antoine eq., Dean 1985, 1992)
243 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.00535 – 1496.2/(–72.15 + T/K); temp range 348–513 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
236 (supercooled liquid P_L, GC-Kovás retention indices correlation; Spieksma et al. 1994)
190.4* (20.39°C, static-pressure gauge, measured range –25 to 159°C, Polednicek et al. 1996)
ln (P/Pa) = 21.6433 – 4031.27/[(T/K) – 47.5846]; temp range 249–432 K (Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
log (P/mmHg) = $3.2904 - 2.5839 \times 10^3/(T/K) + 3.893 \cdot \log (T/K) - 9.5398 \times 10^{-3} \cdot (T/K) + 4.6397 \times 10^{-6} \cdot (T/K)^2$, temp range 248–684 K, (Yaws 1994)
5731* (84.353°C, comparative ebulliometry, measured range 84.353–175.207°C, Roháč et al. 1998)
185.0* (20°C, recommended, summary of literature data, temp range 263.15–463.15 K, Roháč et al. 1999)
$\ln [(P/Pa)/4.85] = [1 - (T/K)/248.39] \cdot \exp\{3.366439 - 8.3811530 \times 10^{-4} \cdot (T/K) + 5.9337577 \times 10^{-7} (T/K)^2\}$; temp range 250–448 K (Cox eq., recommended, Roháč et al. 1999)
log (P/Pa) = 21.6433 – 4031.27/[(T/K) – 47.5846]; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

472 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975; selected exptl., Nirmalakhandan & Speece 1988a)
375 (calculated-bond contribution, Hine & Mookerjee 1975)
182 (20°C, batch air stripping-GC, Oliver 1985)
267 (gas stripping-GC, Warner et al. 1987)
289* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m^3/mol)] = 2.882 – 2564/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
328 (computer value, Yaws et al. 1991)
216 (20°C, equilibrium gas stripping-GC, Hovorka & Dohnal 1997)
269 (21°C, headspace equilibrium-GC, de Wolf & Lieder 1998)
288 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 2.436 – 986/(T/K) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.55 (Hansch et al. 1968)
3.38 (Leo et al. 1971; Hansch & Leo 1979)
3.57, 3.55 (calculated-fragment constants, Rekker 1977)

3.60 (shake flask-GC, Könemann et al. 1979)
3.62 (HPLC-k′ correlation, Könemann et al. 1979)
3.44 (shake flask-LSC, Banerjee et al. 1980)
3.44 (shake flask-LSC, Veith et al. 1980; Oliver & Niimi 1983)
3.95 (HPLC-RT correlation, Veith et al. 1980)
3.53 (shake flask-GC, Watarai et al. 1982)
3.46 (shake flask-HPLC, Hammers et al. 1982)
3.38–3.62, 3.52 (range, mean, shake flask method, Eadsforth & Moser 1983)
3.62–3.95, 3.73 (range, mean, HPLC method, Eadsforth & Moser 1983)
3.48 (generator column-HPLC/UV, Wasik et al. 1983)
3.48 (generator column-GC/ECD, Miller et al. 1984; 1985)
3.57 (HPLC-RV correlation, Garst 1984)
3.60 (Hansch & Leo 1985)
3.55* (19°C, shake flask-GC, measured range 13–33°C, Opperhuizen et al. 1988)
3.50 (shake flask-GC, Pereira et al. 1988)
3.525 (slow stirring, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
3.52 (recommended, Sangster 1993)
3.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.36 (calculated-S_{oct} and vapor pressure, Abraham et al. 2001)
4.27* (20°C, HPLC-k′ correlation, measured range 10–50°C, Su et al. 2002)
log K_{OA} = 57020/(2.303·RT) – 5.856; temp range 10–50°C (HPLC-k′ correlation, Su et al. 2002)

Bioconcentration Factor, log BCF:

1.82 (bluegill sunfish, Veith et al. 1979b; 1980)
1.82 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
2.86 (microorganisms-water, Mabey et al. 1982)
2.57–2.68 mean 2.62; 2.74–2.96 mean 2.87 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
3.70–4.02 (rainbow trout, lipid base, Oliver & Niimi 1983)
2.62–2.87 (fish, Oliver 1984)
1.99 (fathead minnow, flowing water, Carlson & Kosian 1987)
3.77, 3.78, 3.83, 3.84 (13. 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
3.60, 3.86, 3.25, 3.40 (field data-lipid based: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
1.82; 2.62, 2.87 (*Lepomis macrochirus; Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
3.78 (*Poecilla reticulata*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
2.62, 3.70; 2.553, 2.305 (quoted: whole fish, lipid content; calculated-QSPR-MCI χ, K_{OW}, Lu et al. 1999)
3.79; 3.75 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

4.50; 4.10 (field data of sediment trap material; Niagara River-organic matter, Oliver & Charlton 1984)
2.14 (soil, Lee et al. 1989)
2.48 (soil, calculated-QSAR-MCI χ, Sabljic et al. 1995)
2.43, 2.58, 2.88 (RP-HPLC-k′ correlation on three different stationary phases, Szabo et al. 1995)
2.60, 2.60 (RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
3.47 ± 0.74 (suspended particulate in coastal waters, Masunaga et al. 1996)
2.49, 2.53 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:

2.23	(Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm, Chiou et al. 1983)
3.88	(micelle-water, Valsaraj & Thibodeaux 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2}$ = 4.1 h from a model river of 1 m depth with a current of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982);
  $k = 1.9 \times 10^{-4}$ h^{-1} with H_2O_2 at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988);
  pseudo-first-order direct photolysis k(exptl) = (0.008. ± 0.001) min^{-1} with $t_{1/2}$ = (92.3 ± 6.4) min in aqueous solution (Peijnenburg et al. 1992)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
  $k_{OH} \sim 3.0 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
  k << 360 M^{-1} h^{-1} for singlet oxygen and k << 1 M^{-1} h^{-1} for RO_2 radical (Mabey et al. 1982)
  $k_{OH} = (7.2 \pm 0.2) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)
  k_{OH} (obs.) = 7.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1}; and k_{OH}(calc) = 11.5×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1985)
  k_{OH}(calc) = 1.01×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs) = 0.72×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
  k(aq.) = (0.57 ± 0.005) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2}$ = 16 h at pH 7 (Yao & Haag 1991).
  k(aq.) = (5.4–5.9) × 10^{-9} M^{-1} s^{-1} for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)
  $k_{HO\cdot}$(aq.) = (5.0 ± 1.0) × 10^9 M^{-1} s^{-1} in aqueous solutions (Haag & Yao 1992)
  $k_{OH} = 0.46 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982)
  base rate constant k < 0.9 M^{-1} h^{-1} at 25°C with a calculated $t_{1/2}$ > 900 yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)
  first-order $t_{1/2}$ > 879 yr, based on rate constant k < 0.9 M^{-1} h^{-1} extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Howard et al. 1991).

Biodegradation: significant degradation in an aerobic environment with rate constant k = 0.05 d^{-1} (Tabak et al. 1981; Mills et al. 1982);
  nearly 100% removed by an apparent combination of biodegradation and stripping in a continuous flow activated sludge system (Kincannon et al. 1983; selected, Howard 1989)
  $t_{1/2}$(aq. aerobic) = 672–4320 h, estimated from unacclimated soil grab sample data; $t_{1/2}$(aq. anaerobic) = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation: k = 1 × 10^{-10} mL $cell^{-1}$ h^{-1} (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)
  $t_{1/2}$ = 200.6–2006 h, based on photooxidation half-life in air (Howard et al. 1991).

Surface Water: $t_{1/2}$ = 0.9–50 d, various locations in the Netherlands in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980)
  $t_{1/2}$ = 672–4320 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)
  measured rate constant k = (0.57 ± 0.05) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2}$ = 16 h at pH 7 (Yao & Haag 1991)
  direct photolysis $t_{1/2}$ = 92.3 min in aqueous solution (Peijnenburg et al. 1992).

Groundwater: $t_{1/2}$ = 1 yr estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)

$t_{1/2}$ = 1334–8640 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2}$ = 672–4320 h, based on unacclimated aerobic screening test data and aerobic soil grab sample data (Howard et al. 1991).

Biota: $t_{1/2}$ < 1 d in bluegill sunfish (Veith et al. 1980; Barrows et al. 1980)

$t_{1/2}$ < 5 d in worm at 8°C (Oliver 1987a);

biological half-lives, $t_{1/2}$ < 1 d in trout muscle, $t_{1/2}$ < 1 d in sunfish, and $t_{1/2}$ < 1 d in guppy for dichlorobenzenes (Niimi 1987).

TABLE 6.1.1.3.1
Reported aqueous solubilities of 1,3-dichlorobenzene at various temperatures

1.

Klemenc & Löw 1930		Vesala 1973		Schwarz & Miller 1980		Horvath & Getzen 1985	
volumetric method		shake flask-UV spec.		elution chromatography		recommended values	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	111	10	97.63	10	116	10	103
25	123	15.2	97.76	20	89	15	99.9
30	140	19.6	98.32	30	139	20	101
35	150	25.1	101.26	shake flask-UV		25	106
40	167	30.0	112.74	10	120	30	114
45	177	35.0	121.13	20	113	35	125
55	196			30	132	40	137
60	201			average		45	151
				10	118	50	165
				20	101	55	179
				30	135	60	192

2.

Ma et al. 2001		Finizio & Di Guardo 2001	
shake flask-GC		RP-HPLC-k′ correlation	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
5	114	5	71
15	108	15	104
25	126	25	132
35	134	35	166
45	141		

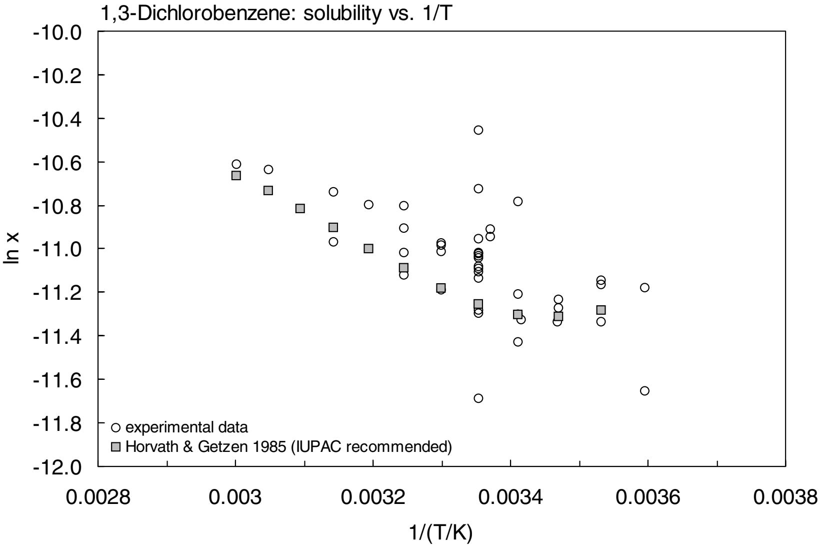


FIGURE 6.1.1.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,3-dichlorobenzene.

TABLE 6.1.1.3.2
Reported vapor pressures of 1,3-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C\cdot\log(T/K)$	(4)		
$\ln(P/P_o) = (1 - T/T_o)\cdot\exp[\Sigma A_iT^i]$	(5) - Cox eq.		

1.

Stull 1947		Dreisbach & Shrader 1949		Polednicek et al. 1996		Roháč et al. 1998	
summary of literature data		ebulliometry		static method-pressure gauge		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.1	133.3	90.72	7605	–23.55	5.459	84.353	5731
39	666.6	98.05	10114	–19.57	7.987	93.65	8343
52.9	1333	111.49	16500	–19.57	7.973	97.99	11076
66.2	2666	140.49	42060	–9.7	19.355	107.17	13922
82	5333	157.37	67660	0.3	44.17	112.433	16799
92.2	7999	173.0	101325	10.34	94.451	117.892	20292
105	13332			10.35	9.459	117.893	20291
125.9	26664	mp/°C	–24.76	20.39	190.4	123.625	24569
149	53329	bp/°C	173.0	30.28	360.02	129.141	29396
173	101325			40.26	652.82	134.535	34819
		eq. 2	P/mmHg	50.15	1122.2	139.715	40761
mp/°C	–24.2	A	7.30364	50.16	1125.0	144.993	47623
		B	1782.4	60.18	1872.9	144.993	47623
		C	230	60.18	1875.7	153.301	60276
				70.03	2980.9	161.253	74765
				70.03	2978.4	169.859	93403
				80.0	4661.7	172.047	98670

(*Continued*)

TABLE 6.1.1.3.2 *(Continued)*

Stull 1947		Dreisbach & Shrader 1949		Polednicek et al. 1996		Roháč et al. 1998	
summary of literature data		ebulliometry		static method-pressure gauge		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				89.94	7042.6	174.92	105933
				89.94	7049.0	175.207	106716
				98.86	10180		
				108.83	14713	bp/°C	173.095
				118.87	20859		
				128.93	28986	eq. 3	P/kPa
				138.94	39411	A	6.16151
				149.05	52842	B	1595.19
				159.06	69604	C	–62.398
				eq. 3a	P/Pa		
				A	21.6433		
				B	4031.27		
				C	–47.5846		

2.

Roháč et al. 1999	
recommended	
T/K	P/Pa
253.15	7.70
263.15	18.9
273.15	43.1
283.15	92.0
283.15	185.0
303.15	352.9
313.15	641.6
232.15	1117
333.15	1871
343.25	3016
353.15	4737
363.15	7205
373.15	10670
383.15	15420
393.15	21810
403.15	30210
413.15	41080
423.15	54920
433.15	72270
443.15	93730
453.15	12000
Cox eq.	
eq. 5	P/Pa
A_0	3.366439
$10^{-4}A_1$	–8.3811530

TABLE 6.1.1.3.2 *(Continued)*

Rohá̆č et al. 1999	
recommended	
T/K	P/Pa
$10^{-7}A_2$	5.9337577
T_o/K	248.39
P_o/Pa	4.85
bp/K	446.25
temp range 250–448 K	

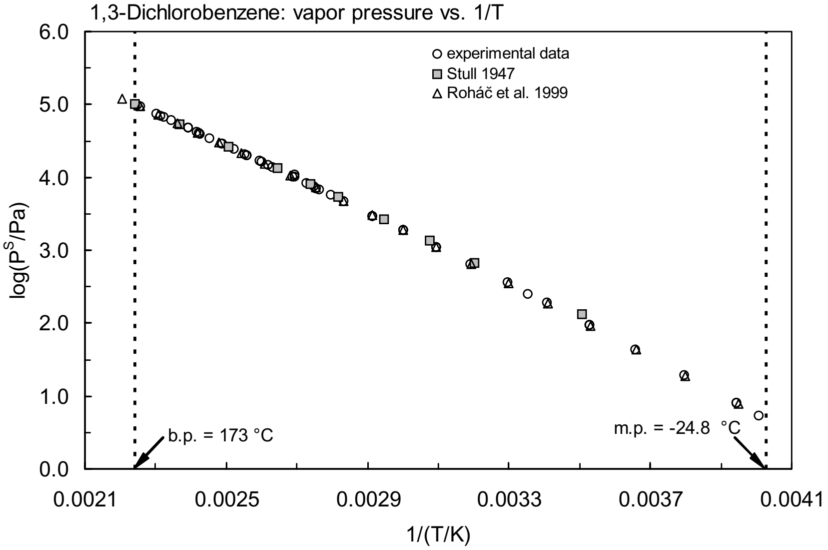


FIGURE 6.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3-dichlorobenzene.

TABLE 6.1.1.3.3
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,3-dichlorobenzene at various temperatures and temperature dependence equations

Henry's law constant		log K_{OW}		log K_{OA}	
Ashworth et al. 2988		Opperhuizen et al. 1988		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OW}	t/°C	log K_{OA}
10	224	13	3.72	10	4.6
15	234	19	3.55	20	4.27
20	298	28	3.48	30	3.96
20	289	33	3.42	40	3.67
30	428			50	3.4
		$\Delta H/(kJ\ mol^{-1}) = -15.0$.			
ln H = A – B/(T/K)				$\Delta H_{OA}/(kJ\ mol^{-1}) = 57.02$	
	H/(atm m³/mol)				
A	–2.882			log K_{OA} = A + B/2.303RT	
B	2564			A	–5.856
				B	57020

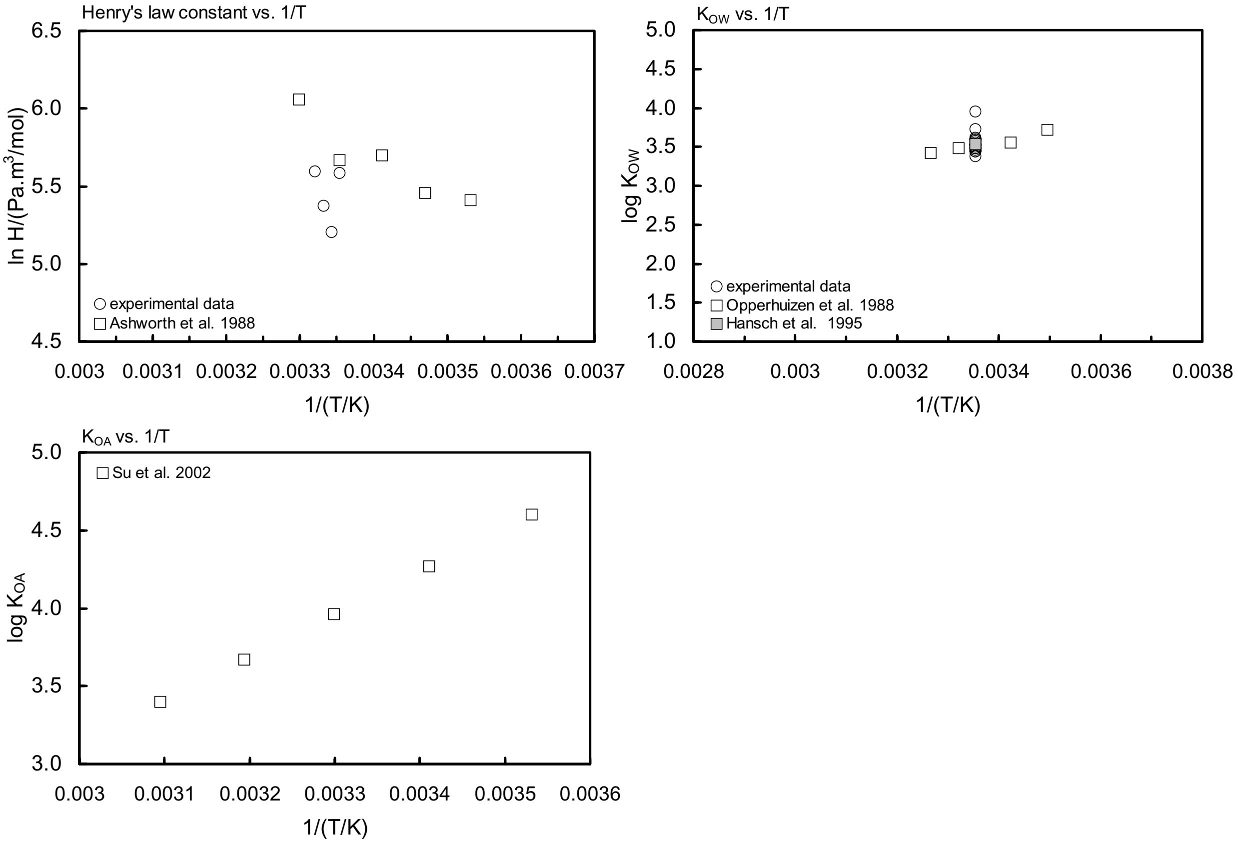
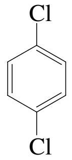


FIGURE 6.1.1.3.3 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for 1,3-dichlorobenzene.

6.1.1.4 1,4-Dichlorobenzene



Common Name: 1,4-Dichlorobenzene
Synonym: *p*-dichlorobenzene, paradichlorobenzene
Chemical Name: 1,4-dichlorobenzene
CAS Registry No: 106-46-7
Molecular Formula: $C_6H_4Cl_2$
Molecular Weight: 147.002
Melting Point (°C):
  53.09 (Lide 2003)
Boiling Point (°C):
  174 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.2457 (Dreisbach 1955; Weast 1972–73; Horvath 1982)
Molar Volume (cm^3/mol):
  118.0 (20°C, calculated-density)
  137.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  18.72 (Dreisbach 1955)
  17.882 (Weast 1972–73)
  18.16, 18.70 (Wauchope & Getzen 1972)
  18.20 (Tsonopoulos & Prausnitz 1971; Dean 1985)
  19.0 (Miller et al. 1984)
  17.153 (Ruelle et al. 1993)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  56.484 (Pirsch 1956)
  55.65 (Tsonopoulos & Prausnitz 1971)
  54.81 (Weast 1976–77; Amidon & Williams 1982; Yalkowsky 1979)
  56.07 (Yalkowsky & Valvani 1980)
  58.16 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.53 (mp at 53.09°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  79.1* (volumetric method, measured range 20–60°C, Klemenc & Löw 1930)
  77 (30°C, shake flask-interferometer, Gross & Saylor 1930)
  < 500 (residue-volume method, Booth & Everson 1948)
  76 (shake flask-UV, Andrew & Keefer 1950)
  89.8 (Landolt-Börnstein 1951)
  83.4* (24.6°C, shake flask-UV, measured 22.2–73.4°C, Wauchope & Getzen 1972)
  85.5 (shake flask-UV, Vesala 1974)
  56.9 (20°C, shake flask-GC/ECD, Chiou & Freed 1977)
  34 (shake flask-GC, Jones et al. 1977/1978)
  87.2 (shake flask-GC, Aquan-Yuen et al. 1979)
  90.6 (shake flask-UV, Yalkowsky et al. 1979)
  73.7 (shake flask-LSC, Veith et al. 1980)
  73.8 (shake flask-LSC, Banerjee et al. 1980)
  48.7 (shake flask-GC, Könemann 1981)
  73, 137 (shake flask-GC, solid, supercooled liquid, Chiou et al. 1982)

90.0 (recommended, Horvath 1982)

25 (calculated-UNIFAC activity coefficients, Arbuckle 1983)

175 (calculated-HPLC-k′, converted from reported γ_W, Hafkenscheid & Tomlinson 1983a)

154 (30°C, shake flask-GC, McNally & Grob 1983)

30.9 (generator column-GC, Miller et al. 1984, 1985)

65.3 (shake flask-HPLC, Banerjee 1984)

158 (30°C, shake flask-GC, McNally & Grob 1984)

82.9* (recommended, temp range 10–75°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(g/kg) = 13.974 - 8.5829 \times 10^{-2} \cdot (T/K) + 1.3365 \times 10^{-4} \cdot (T/K)^2$; temp range 328–348 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

100 (Dean 1985)

141 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

81.4* ± 1.5 (shake flask-GC/ECD, measured range 5–45°C, Shiu et al. 1997)

42.0 (shake flask-GC, Boyd et al. 1998)

$\ln x = -4.178 - 2186.7/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1333* (54.8°C, summary of literature data, temp range 54.8–173.9°C, Stull 1947)

$\log (P/mmHg) = 7.30697 - 1788.7/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)

7605* (92.0°C, ebulliometry, measured range 92.0–174.12°C, Dreisbach & Shrader 1949)

235 (calculated by formula., Dreisbach 1955; quoted, Hine & Mookerjee 1975; Riddick et al. 1986; Howard 1989)

$\log (P/mmHg) = 6.89797 - 1507.3/(201.0 + t/°C)$; temp range 75–240°C (Antoine eq. for liquid state, Dreisbach 1955)

8514* (94.8°C, ebulliometry, measured range 94.8–174.04°C, McDonald et al. 1959)

93.33* (20.4°C, α–*p*-dichlorobenzene, manometry, measured range 20.4–39.6°C, Walsh & Smith 1961)

402.6* (37.9°C, β-*p*-dichlorobenzene, manometry, measured range 37.9–52.5°C, Walsh & Smith 1961)

90.2 (solid vapor pressure, extrapolated, Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 17260.5/(T/K)] + 12.4800$; temp range 30–50°C, (Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 10611.0/(T/K)] + 8.073632$; temp range 54.8–173.9°C (Antoine eq., Weast 1972–73)

137.2* (diaphragm pressure gauge, measured range: 0–20°C, De Kruif et al. 1981)

128 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.94201 - 1668.355/(186.212 + t/°C)$; temp range 164.7–237.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

158* (gas saturation-GC, measured range 20–100°C, Rordorf 1985)

243 (extrapolated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 7.0208 - 1590.9/(210.2 + t/°C)$, temp range 95–174°C (Antoine eq., Dean 1985, 1992)

86.7 (20°C, gas saturation, Chiou & Shoup 1985)

134 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 10.472 - 3382.9/(T/K)$; temp range 293–313 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 10.181 - 3290.4/(T/K)$; temp range 310–336 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.12695 - 1578.51/(-64.22 + T/K)$; temp range 341–448 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

133* (gas saturation-GC, measured range –15 to 40°C, Liu & Dickhut 1994)

216; 257 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)

$\log (P/mmHg) = 36.2276 - 3.6756 \times 10^3/(T/K) - 9.6308 \cdot \log (T/K) - 1.3372 \times 10^{-9} \cdot (T/K) + 1.9905 \times 10^{-6} \cdot (T/K)^2$; temp range 326–685 K (vapor pressure eq., Yaw et al. 1994)

135* (25°C; pressure gauge measurement; interpolated from reported Antoine eq., Polednicek et al. 1996)

$\ln (P_S/Pa) = 28.4986 - 6272.86/[(T/K) - 32.2741]$; temp range 273–323 K (Antoine eq. from exptl data, pressure gauge measurement, solid, Polednicek et al. 1996)

$\ln (P_L/Pa) = 21.0472 - 3665.96/[(T/K) - 62.3849]$; temp range 333–442 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Polednicek et al. 1996)

5729* (85.139°C, comparative ebulliometry, measured range 85.139–175.626°C, Roháč et al. 1998)
87.0* (20°C, recommended, summary of literature data, temp range 273.15–453.15 K, Roháč et al. 1999)
$\ln [(P_S/\text{Pa})/1280] = [1 - (T/\text{K})/326.3]\cdot\exp\{3.251427 - 2.853921 \times 10^{-4}\cdot(T/\text{K})\}$; temp range 273–323 K (Cox eq. solid, recommended, Roháč et al. 1999)
$\ln [(P_L/\text{Pa})/1280] = [1 - (T/\text{K})/326.3]\cdot\exp\{3.100023 - 1.0557743 \times 10^{-3}\cdot(T/\text{K}) + 7.816354 \times 10^{-7}(T/\text{K})^2\}$; temp range 328–449 K (Cox eq., liquid, recommended, Roháč et al. 1999)
$\log (P/\text{Pa}) = 11.63209 - 2829.32/(T/\text{K})$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

330 (equilibrium cell-GC, concentration ratio, Leighton & Calo 1981)
240 (gas stripping-GC, Mackay & Shiu 1981)
152 (20°C, gas stripping-GC, Oliver 1985)
276 (gas stripping-GC, Warner et al. 1987)
321* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 3.373 - 2720/(T/\text{K})$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
438 (computer value, Yaws et al. 1991)
244 (gas stripping-GC, Shiu & Mackay 1997)
188 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
275 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 2.649 - 1054/(T/\text{K})$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

3.39 (shake flask, Leo et al. 1971; Hansch & Leo 1979)
3.57, 3.55 (calculated-fragment constants, Rekker 1977)
3.38 (Hansch & Leo 1979)
3.62, 3.39 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
3.37, 3.78 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
3.37 (shake flask-LSC, Banerjee et al. 1980)
3.46 (HPLC-k′ correlation, Hammers et al. 1982)
3.52 (shake flask-GC, Watarai et al. 1982)
3.43 (HPLC-k′ correlation, Miyake & Terada 1982)
3.67, 3.90 (calculated-UNIFAC activity coefficients, Arbuckle 1983)
3.37 (generator column-HPLC/UV, Wasik et al. 1983)
3.38 (generator column-GC/ECD, Miller et al. 1984; 1985)
3.37 (HPLC-RV correlation, Garst 1984; Garst & Wilson 1984)
3.52 (Hansch & Leo 1985)
3.444 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
3.85–4.30, 4.0 (range, average: round robin work, shake flask or HPLC-k′ correlation, Kishi & Hashimoto 1989)
3.355 ± 0.053, 3.444 ± 0.001 (shake flask methods, interlaboratory studies, Brooke et al. 1990)
3.45 (recommended, Sangster 1993)
3.44 (recommended, Hansch et al. 1995)
3.23* ± 0.03 (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)
$\log K_{OW} = 0.2338 + 17100/[2.303\cdot R(T/\text{K})]$; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
3.65 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.46 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)
4.32* (20°C, HPLC-k′ correlation, measured range 10–50°C, Su et al. 2002)
$\log K_{OA} = 55590/(2.303\cdot RT) - 5.556$; temp range 10–50°C (HPLC-k′ correlation, Su et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

2.33 (rainbow trout, Neely et al. 1974)
2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
1.78 (bluegill sunfish, Veith et al. 1979b, 1980)
1.78 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
3.26 (guppy, lipid basis, Könemann & van Leeuwen 1980)
2.53–2.59 mean 2.57; 2.79–2.96 mean 2.86 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
3.64–3.96 (rainbow trout, lipid basis, Oliver & Niimi 1983)
3.40 (15°C, guppy, Banerjee et al. 1984)
2.83–2.86 (fish, Oliver 1984)
2.00, 1.70, 2.75 (algae, fish, activated sludge, Freitag et al. 1984)
2.0, 1.70, 2.75 (algae, fish, activated sludge, Freitag et al. 1985)
2.32–2.72 mean 2.71; 2.74–3.15 mean 2.95 (15°C, rainbow trout, wet wt., steady-state BCF on 7- to 96-d laboratory study in two tanks with different water concn, Oliver & Niimi 1985)
2.04 (fathead minnow, flowing water, Carlson & Kosian 1987)
5.3–5.6, 5.5 (Niagara River plume, range, mean; Oliver 1987b)
3.91, 4.53, 4.09, 3.51 (field data-lipid based: Atlantic creakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.25 (guppy, lipid weighted-based, 12 to 31 d exposure-GC, Gobas et al. 1989)
2.47, 3.56 (flagfish: whole fish, lipid, Smith et al. 1990)
1.7 ± 0.2 (guppy, steady-state conditions, rate const. ratio k_1/k_2, 96-h exposure, Sijm et al. 1993)
3.5 ± 0.1 (guppy, lipid normalized BCF, Sijm et al. 1993)
2.40 (fathead minnow, steady-state conditions, rate const. ratio k_1/k_2, 96-h exposure, Sijm et al. 1993)
3.60 (fathead minnow, lipid normalized BCF, Sijm et al. 1993)
1.78; 2.47; 2.57–2.95 (*Lepomis macrochirus; Jordanella floridae; Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
1.70; 2.40 (*Poecilla reticulata; Pimephales promelas*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
2.57, 3.65; 2.517, 2.242 (quoted: whole fish, lipid content; calculated-MCI χ, K_{OW}, Lu et al. 1999)
3.70; 3.75 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

2.59 (Kenaga 1980a)
2.78–3.14 (organic carbon, Schwarzenbach & Westall 1981)
2.29 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
2.18–3.44 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
4.80; 5.00 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
2.82, 2.45 (Aprison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium Southworth & Keller 1986)
5.30–5.60; 5.50 (Niagara River plume: range; average value; Oliver 1987b)
2.92; 2.91 (Aldrich humic acid, equilibrium dialysis; Aldrich and Fluka humic acid, Flory-Huggins model, Chin & Weber 1989)
2.43 (organic polymers in Huran River water, Chin et al. 1990)
2.88 (HPLC-k′ correlation, Szabo et al. 1995)
2.60, 2.61 (RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.66, 2.57, 2.77 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
2.99–3.46 (three wetland soils, batch equilibrium-sorption isotherm-LSC, Lee et al. 2003)

Sorption Coefficient, log K_{OM}:

2.20 (Woodburn silt loam soil, organic matter 1.9%, equilibrium sorption isotherm, Chiou et al. 1983)

Environmental Fate Rate Constants, k or Half-Lives. $t_{½}$:

Volatilization: $t_{½}$ = 4.3 h from a model river of 1 m depth and with a current of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982);

rate constants: k = 0.04 d^{-1}, $t_{½}$ = 18 d in spring at 8–16°C, k = 0.068 d^{-1}, $t_{½}$ = 10 d in summer at 20–22°C, k = 0.054 d^{-1}, $t_{½}$ = 13 d in winter at 3–7°C for the periods when volatilization appears to dominate, and k = 0.066 d^{-1}, $t_{½}$ = 10.6 d with $HgCl_2$, and k = 0.063 d^{-1}, $t_{½}$ = 11 d without $HgCl_2$ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982)

Direct photolysis unimportant (Zepp & Cline 1977; Zepp 1978);

$t_{½}$ = 25 d under sunlight in water (Mansour & Feicht 1994)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k = 9.63×10^{-3} h^{-1} in air (Ware & West 1977; selected, Mackay et al. 1985)

k_{OH} ~ 3.0×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

k << 360 M^{-1} h^{-1} for singlet oxygen and k << 1 M^{-1} h^{-1} for RO_2 radical (Mabey et al. 1982)

k << 3 M^{-1}·s^{-1} for the reaction with ozone in water using 0.5 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

k_{OH} = $(3.2 \pm 0.2) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

k_{OH} (obs.) = 3.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1}; and k_{OH}(calc) = 4.9×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1985)

k_{OH}(calc) = 0.41×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs) = 0.32×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH} = $(0.32 - .52) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295–300 K (literature review, Atkinson 1989)

$t_{½}$ = 200.6–2006 h based on vapor phase reaction with OH radicals (Howard et al. 1991)

k = $(5.0 - 5.3) \times 10^9$ M^{-1} s^{-1} for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{HO\cdot}$ = 4.0×10^9 $M^{-1}s^{-1}$ in aqueous solutions (Haag & Yao 1992)

k_{OH}(calc) = 0.44×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993).

Hydrolysis: not environmentally significant (Mabey et al. 1982);

base rate constant k < 0.9 M^{-1} h^{-1} at 25°C with a calculated $t_{½}$ > 900 yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

first order $t_{½}$ > 879 yr, based on rate constant k < 0.9 M^{-1} h^{-1} extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Howard et al. 1991).

Biodegradation:

k = 1.09×10^{-2} h^{-1} degradation in water (Verschueren 1977)

$t_{½}$(aq. aerobic) = 672–4320 h, based on unacclimated aerobic screening test data (Canton et al. 1985) and aerobic soil grab sample data (Haider et al. 1981; Howard et al. 1991)

k = 0.05 d^{-1}, significant degradation in aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$t_{½}$(aq. anaerobic) = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: 1×10^{-10} mL $cell^{-1}$ h^{-1} (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 5.67 h^{-1}; k_2 = 0.0264 h^{-1} (trout muscle, Neely et al. 1974; Neely 1979)

k_1 = 7.44 h^{-1} (10°C, yellow perch, Neely et al. 1974; Neely 1979)

k_1 = 17.0 h^{-1} (25°C, yellow perch, Neely et al. 1974; Neely 1979)

kk_1 = 1800 d^{-1}; k_2 = 1.00 d^{-1} (guppy, Könemann & van Leeuwen 1980)

k_1 = 4.1 h^{-1}; $1/k_2$ = 24 h (guppy, quoted from Könemann & van Leeuwen 1980, Hawker & Connell 1985)

k_1 = 5.7 h^{-1}; $1/k_2$ = 38 h (rainbow trout, quoted from Neely et al. 1974, Hawker & Connell 1985)

k_1 = 97 d^{-1} (fish, quoted, Opperhuizen 1986)

log k_2 = 0, –0.2 d^{-1} (fish, calculated-K_{OW}, Thomann 1989)

log k_1 = 1.99 d^{-1}; log k_2 = 0.0 (guppy, 12–31 d exposure experiments, Gobas et al. 1989)

log k_1 = 1.99 d^{-1} (fish, quoted, Connell & Hawker 1988)

k_1 = 291 d^{-1}, 4230 d^{-1}; k_2 = 0.98 d^{-1}, 1.18 d^{-1} (American flagfish: whole fish, fish lipid, Smith et al. 1990)

k_2 = 0.98 d^{-1}, 1.46 d^{-1} (American flagfish: bioconcentration exptl., toxicity data, Smith et al. 1990)
k_1 = 760 L kg^{-1} d^{-1}; k_2 = 4.80 d^{-1} (guppy, 96-h exposure, Sijm et al. 1993)
k_1 = 600 L kg^{-1} d^{-1}; k_2 = 2.50 d^{-1} (fathead minnow, 96-h exposure, Sijm et al. 1993)

Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$t_{1/2}$ = 200.6–2006 h, based on photooxidation half-life in air (Howard et al. 1991)

Surface Water:
$t_{1/2}$ = 1.1–26 d, various locations in the Netherlands in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980);
half-lives from marine mesocosm: $t_{1/2}$ = 18 d in the spring at 8–16°C, $t_{1/2}$ = 10 d in the summer at 20–22°C and $t_{1/2}$ = 31 d in the winter at 3–7°C when volatilization dominates, and $t_{1/2}$ = 10.6 d and 11 d for experiments with and without $HgCl_2$, respectively, in September 9–15 (Wakeham et al. 1983);
hydrolysis $t_{1/2}$ > 900 yr at pH 7 and 25°C (Ellington et al. 1988)
$t_{1/2}$(aerobic) = 672–4320 h, based on unacclimated aerobic screening test data and aerobic soil grab sample data; $t_{1/2}$(anaerobic) = 2688–17280 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
photolysis $t_{1/2}$ = 25 d under sunlight in water (Mansour & Feicht 1994).

Groundwater: $t_{1/2}$ ~1 yr estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)
$t_{1/2}$ = 1344–8640 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2}$ = 672–4320 h, based on unacclimated aerobic screening test data and aerobic soil grab sample data (Howard et al. 1991).

Biota: $t_{1/2}$ < 1 d in fish tissues (Veith et al. 1980);
$t_{1/2}$ < 1 d in bluegill sunfish (Barrows et al. 1980);
$t_{1/2}$ = 16 h, clearance from fish (Neely 1980);
$t_{1/2}$ < 5 d in worms at 8°C (Oliver 1987a);
biological half-lives, $t_{1/2}$ < 1 d in trout muscle, $t_{1/2}$ < 1 d in sunfish and $t_{1/2}$ < 1 d in guppy for dichlorobenzenes (Niimi 1987);
depuration $t_{1/2}$ = 0.70 d for whole fish, $t_{1/2}$ = 0.59 d for fish lipid (American flagfish, Smith et al. 1990).

TABLE 6.1.1.4.1
Reported aqueous solubilities of 1,4-dichlorobenzene at various temperatures

Klemenc & Löw 1930		Wauchope & Getzen 1972		Horvath & Getzen 1985		Shiu et al. 1997	
volumetric method		shake flask-UV		recommended values		shake flask-GC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
		liquid		liquid			
20	68.1	22.2	77.8	10	51.2	5	48.6
20	79.1	24.6	83.4	15	60.5	15	63.0
30	93.3	25.5	86.9	20	71.0	25	81.4
35	104	30.0	92.6	25	82.9	35	104.5
35	83	34.5	102	30	96.3	45	130
40	101	38.4	121	35	111.3		
45	122	47.5	169	40	128		
55	156	50.1	173	45	147		
60	163	solid		30	167		
		59.2	210	55	190		
		60.7	218	solid			
		65.1	230	55	201		
		65.2	237	60	214		
		73.4	281	65	233		
				70	259		
				75	292		

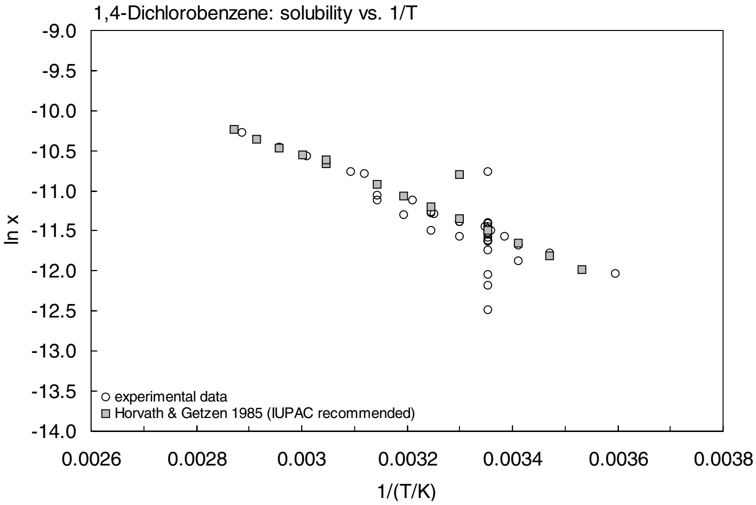


FIGURE 6.1.1.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,4-dichlorobenzene.

TABLE 6.1.1.4.2
Reported vapor pressures of 1,4-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\quad \ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\quad \ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3) $\quad \ln P = A - B/(C + T/K)$ (3a)
$\log P = A - B/(T/K) - C \cdot \log(T/K)$ (4)
$\ln(P/P_o) = (1 - T/T_o) \cdot \exp[\Sigma A_i T^i]$ (5) - Cox eq.

1.

Stull 1947		**Dreisbach & Shrader 1949**		**McDonald et al. 1959**		**Walsh & Smith 1961**	
summary of lit. data		**ebulliometry**		**ebulliometry**		**manometry**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
						α-*p*-dichlorobenzene	
54.8	1333	92.0	7605	94.8	8514	20.4	93.33
69.2	2666	99.41	10114	98.55	9844	23.9	121.32
84.8	5333	112.66	16500	104.81	12444	26.8	156.0
95.2	7999	141.65	42066	116.28	18808	29.8	202.65
108.4	13332	158.52	67660	143.52	44465	33.2	269.3
128.3	26664	174.12	101325	159.79	70117	33.7	277.3
150.2	53329			171.87	95945	35.0	312.0
173.9	101325			174.04	101325	36.4	317.3
						37.3	350.6
mp/°C	53.0			mp/°C	52.90	37.5	382.6
						39.2	440.0
				eq. 2	P/mmHg	39.6	454.6
				A	6.99800		
				B	1575.11	mp/°C	53.23
				C	208.513		
						eq. 1	P/mmHg
						A	11.347
						B	3382.9
						$\Delta H_{subl}/(kJ\ mol^{-1})$ = 64.79	

2.

Walsh & Smith 1961		**de Kruif et al. 1981**		**Rordorf 1985**		**Liu & Dickhut 1994**	
manometry		**static manometry**		**gas saturation**		**gas saturation-GC**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
β-*p*-dichlorobenzene							
37.9	402.6	1.47	14.14	25	158.1*	–14.5	4.67
39.8	469.3	3.94	18.32	50	1217.6*	–5.0	16.0
40.2	477.3	6.45	23.67	75	6992.7	10	31.7
40.5	490.6	8.43	28.88	100	31774	25	133
40.8	501.3	10.33	34.83	125	119380	40	452
41.1	508.0	12.35	42.44	150	383592		
41.3	522.6	14.3	51.13				
41.7	534.6	16.63	63.79				
42.4	568.0	19.84	85.98		*solid		
42.6	584.0			eq. 1	P/Pa	$\Delta H_V/(kJ\ mol^{-1})$ = 35.0	
42.9	593.3			A	13.384		
43.2	597.3	eq. 1	P/Pa	B	3450		

TABLE 6.1.1.4.2 *(Continued)*

Walsh & Smith 1961		de Kruif et al. 1981		Rordorf 1985		Liu & Dickhut 1994	
manometry		static manometry		gas saturation		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
43.7	629.3	A	13.6459				
44.1	640.0	B	3431.3		liquid		
45.8	727.9			eq. 1	P/Pa		
46.4	766.6			A	10.472		
48.0	859.3	$\Delta H_{subl}/(kJ\ mol^{-1}) = 65.7$		B	3382.9		
49.4	955.9		11°C				
51.3	955.9			$\Delta H_{subl}/(kJ\ mol^{-1}) = 65.40$			
51.7	1135			30–50°C			
52.5	1192						
eq. 1	P/mmHg						
A	11.056						
B	3290.4						
$\Delta H_{subl}/(kJ\ mol^{-1}) = 63.01$							

3.

Polednicek et al. 1996				Roháč et al. 1998		Roháč et al. 1999	
pressure gauge				comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
	solid		liquid				
0.34	12.2	60.12	1838.2	85.139	5729	273.15	12.2
0.35	11.98	60.15	1839.6	94.305	8334	283.15	33.8
10.35	34.25	70.03	2948.1	101.656	11074	283.15	87.0
10.35	34.21	80.03	4629.1	107.836	13921	303.15	209.3
20.35	88.75	80.04	4627.7	113.103	16800	313.15	474.2
20.35	88.61	89.99	7038.6	118.564	20290	232.15	1017
30.31	214.6	90.0	7041.4	118.568	20292	333.15	1817
40.25	485.5	98.72	9904.2	124.29	24570	343.25	2941
50.15	1037	108.68	1434.2	129.822	29388	353.15	4611
25	135.0	118.73	20385	135.223	34809	363.15	7020
	interpolated	128.78	28351	140.416	40752	373.15	10410
		138.8	38541	145.702	47615	383.15	15060
for solid:		148.28	51728	154.032	60269	393.15	21310
eq. 3a	P/Pa	158.9	68186	154.033	60271	403.15	29550
A	28.4986	168.93	88642	162.009	74759	413.15	40220
B	6272.86			170.622	93393	423.15	53800
C	–32.2741			172.86	98793	433.15	70850
		for liquid:		175.626	105783	443.15	91950
		eq. 3a	P/Pa			453.15	11780
		A	21.0472	bp/°C	173.864		
		B	3665.96			Cox eq.	for solid
		C	–62.3849	eq. 3	P/kPa	eq. 5	P_S/Pa
				A	6.13050	A_0	3.251427
				B	1575.69	$10^{-4}A_1$	–2.8153921
				C	–65.007	A_2	0
						temp range 273–323 K	

(Continued)

TABLE 6.1.1.4.2 (*Continued*)

Polednicek et al. 1996				Roháč et al. 1998		Roháč et al. 1999	
pressure gauge				comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						eq. 5	P_L/Pa
						A_0	3.100023
						$10^{-3}A_1$	–1.0557743
						$10^{-7}A_2$	7.8161354
						T_o/K	326.3
						P_o/Pa	1280.0
						bp/K	447.01
						temp range 328–449 K	

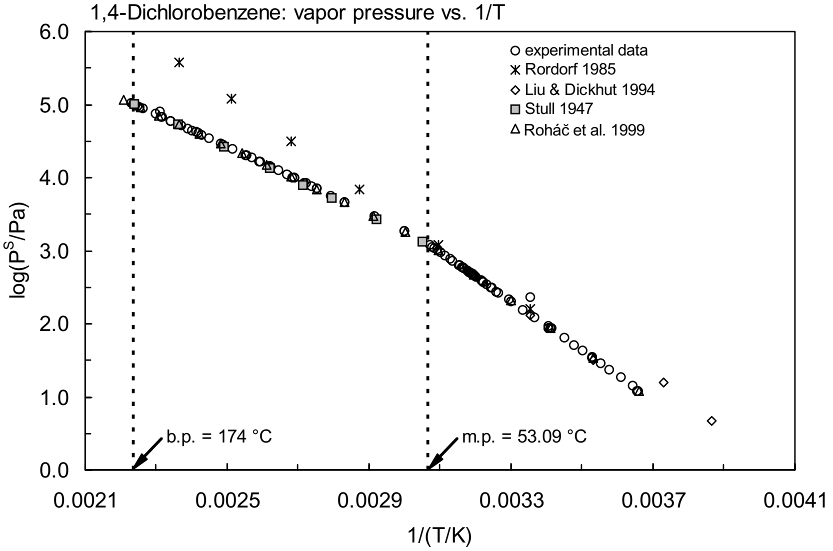


FIGURE 6.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for 1,4-dichlorobenzene.

TABLE 6.1.1.4.3
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,4-dichlorobenzene at various temperatures

Henry's law constant		log K_{OW}		log K_{OA}	
Ashworth et al. 1988		Bahadur et al. 1997		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OW}	t/°C	log K_{OA}
10	215	5	3.42	10	4.65
15	220	15	3.35	20	4.32
20	262	25	3.23	30	4.01
20	321	35	3.12	40	3.72
30	394	45	3.03	50	3.45

TABLE 6.1.1.4.3 (*Continued*)

Henry's law constant		log K_{OW}		log K_{OA}	
Ashworth et al. 1988		Bahadur et al. 1997		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
t/°C	H/(Pa m^3/mol)	t/°C	log K_{OW}	t/°C	log K_{OA}
ln H = A – B/(T/K)		enthalpy of transfer		ΔH_{OA}/(kJ mol^{-1}) = 55.59	
	H/(atm m^3/mol)	ΔH/(kJ mol^{-1}) = –17.1			
A	3.373			log K_{OA} = A + B/2.303RT	
B	2720	log K_{OW} = A – ΔH/2.303RT		A	–5.556
		A	0.2338	B	55590
		ΔH	–17100		

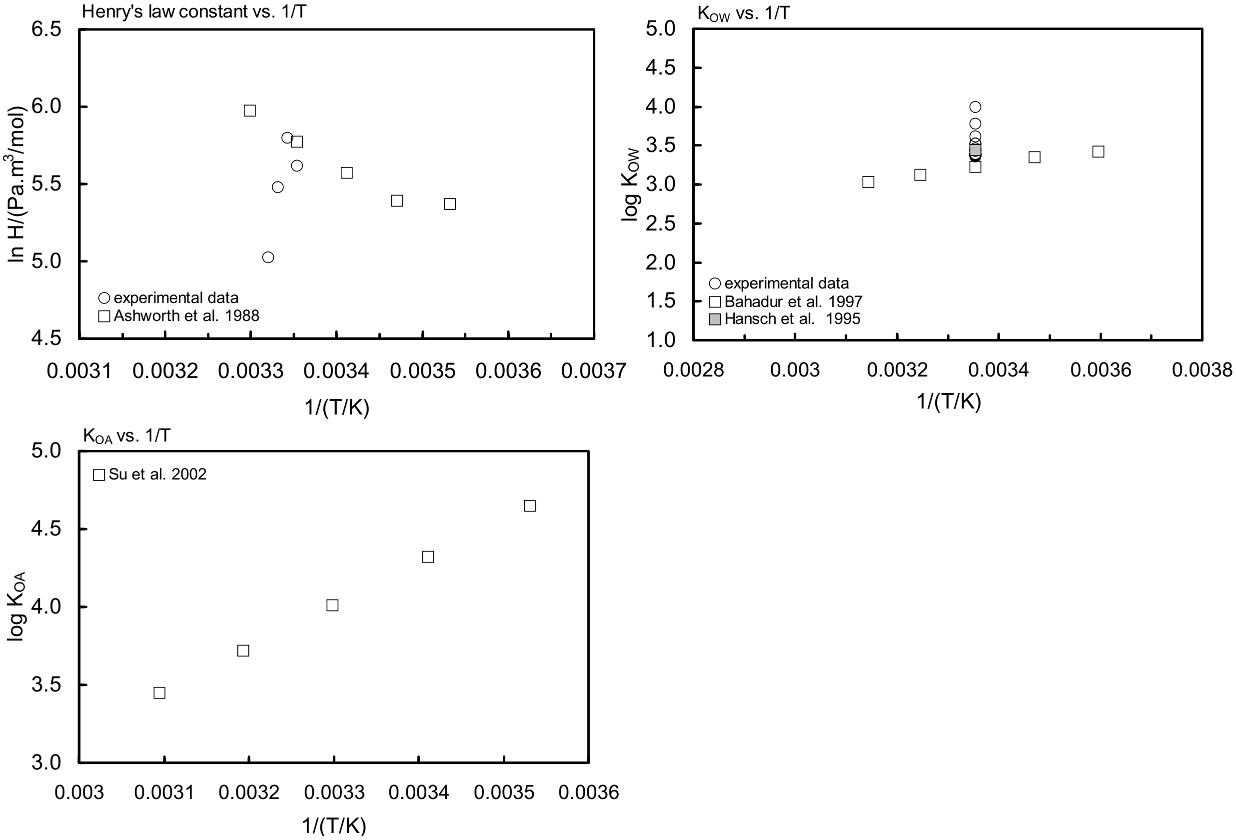
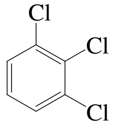


FIGURE 6.1.1.4.3 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for 1,4-dichlorobenzene.

6.1.1.5 1,2,3-Trichlorobenzene



Common Name: 1,2,3-Trichlorobenzene
Synonym: vic-trichlorobenzene
Chemical Name: 1,2,3-trichlorobenzene
CAS Registry No: 81-61-6
Molecular Formula: $C_6H_3Cl_3$
Molecular Weight: 181.447
Melting Point (°C):
51.3 (Lide 2003)
Boiling Point (°C):
218.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.4533 (40°C, Weast 1972–73; Horvath 1982)
1.4533 (25°C, Lide 2003)
1.69 (Dean 1985, 1992)
Molar Volume (cm^3/mol):
124.9 (25°C, calculated-density)
158.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.364 (Tsonopoulos & Prausnitz 1971)
17.99 (Miller et al. 1984)
17.153 (Ruelle et al. 1993)
20.50 (Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.14 (Tsonopoulos & Prausnitz 1971)
56.90 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.552 (mp at 51.3°C)
0.53 (25°C, mp at 53°C, Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
25.1 (Tsonopoulos & Prausnitz 1971)
31.5 (shake flask-UV, Yalkowsky et al. 1979, 1983)
16.6 (shake flask-GC, Mackay & Shiu 1981)
12.0 (shake flask-GC, Könemann 1981)
31.6 (recommended, Horvath 1982)
12.27 (generator column-GC/ECD, Miller et al. 1984, 1985)
18.0 (shake flask-HPLC, Banerjee 1984)
16.3 (23°C, shake flask-GC, Chiou 1985)
18.0 (shake flask-GC, Chiou et al. 1986; Chiou et al. 1991)
19.3* ± 0.24; 23.7 ± 1.3 (generator column-GC/ECD; shake flask-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
13.0 (shake flask-GC, Boyd et al. 1998)
$\ln x = -1.773 - 3418.9/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
19.71, 14.8, 21.04, 40.25 (5, 15, 25, 35°C, estimated- RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (40°C, summary of literature data, Stull 1947)

52.4 (extrapolated-Antoine eq., supercooled liquid P_L, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 11349.5/(T/K)] + 7.91649; temp range 40–218.5°C (Antoine eq., Weast 1972–73)
28.0 (selected-converted from reported P_L, with fugacity ratio, Mackay & Shiu 1981)
25.1 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
17.7 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 9.787 – 3440/(T/K); temp range 289–303 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.23008 – 2624.09/(10.506 + T/K); temp range 343–492 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
11.20* (gas saturation-GC, measured range –15 to 40°C, Liu & Dickhut 1994)
8.82* (20.35°C, static method-pressure gauge measurement; Antoine eq., measured range 0.36–169°C, Polednicek et al. 1996)
ln (P_S/Pa) = 33.2977 – 9327.37/[(T/K) + 6.13445]; temp range 272–3 (Antoine eq. from exptl data, pressure gauge measurement, solid, Polednicek et al. 1996)
ln (P_L/Pa) = 21.1681 – 4077.21/[(T/K) – 71.6539]; temp range 334–2 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Polednicek et al. 1996)
44.1 (supercooled liquid P_L, GC-Kovás retention indices correlation; Spieksma et al. 1994)
8.50* (20°C, recommended, summary of literature data, temp range 233.15–503.15 K, Roháč et al. 1999)
ln [(P_S/Pa)/173.0] = [1 – (T/K)/325.6)·exp{3.380608 – 2.5802866 × 10^{-4}·(T/K)}; temp range 273–323 K (Cox eq., solid, recommended, Roháč et al. 1999)
ln [(P_L/Pa)/173.0] = [1 – (T/K)/325.6)·exp{3.274398 – 1.0923018 × 10^{-3}·(T/K) + 7.8603029 × 10^{-7}(T/K)^2}; temp range 333–448 K (Cox eq., liquid, recommended, Roháč et al. 1999)
log (P/kPa) = 9.787 – 3440/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
127 (gas stripping-GC, Mackay & Shiu 1981)
90.0 (gas stripping-GC, Oliver 1985)
72.0 (20°C, gas stripping-GC, ten Hulscher et al. 1992)
147 (equilibrium air stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
4.27 (Leo et al. 1971; Hansch & Leo 1979)
4.11, 3.99 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
4.02 (HPLC-k′ correlation, McDuffie 1981)
3.97 (shake flask-GC, Watarai et al. 1982)
3.96 (HPLC-k′ correlation, Hammers et al. 1982)
4.04 (generator column-GC, Miller et al. 1984, 1985)
4.14 (shake flask-GC, Chiou 1985)
4.14 (shake flask-GC, Pereira et al. 1988)
4.139 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
4.05 (recommended, Sangster 1993)
4.14 (recommended, Hansch et al. 1995)
3.81* (estimated- RP-HPLC-k′ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
5.19*, 5.11 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
6.491, 6.073, 5.699, 5.385 (–10, 0, 9.88, 19.85°C, generator column-GC, Harner & Mackay 1995)
log K_{OA} = –4.6 + 20–8.7/(T/K); ΔH_{OA} = 55.7 kJ/mol (Harner & Mackay 1995)
5.19 (calculated-S_{oct} and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
4.11 (guppy, lipid basis, Könemann & van Leeuwen 1980)
3.00–3.20 mean 3.08; 3.34–3.52 mean 3.41 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

4.15–4.47 (rainbow trout, lipid basis, Oliver & Niimi 1983)
3.08–3.42 (fish, Oliver 1984)
4.35 (rainbow trout, hatching, 3.2% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
4.11 (guppy, 5.4% lipid, wet wt basis, Geyer et al. 1985)
4.11 (guppy, lipid weight base, 12 to 31-d exposure studies, Gobas et al. 1987, 1989)
2.85 (fish, calculated-concentration ratio C_B/C_W or rate constant ratio k_1/k_2, Connell & Hawker 1988)
3.28 (guppy, Van Hoogan & Opperhuizen 1988)
4.76, 4.90, 3.54, 4.68 (field data-lipid based: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.30 (guppy, steady-state conditions, rate const. ratio k_1/k_2, 96-h exposure, Sijm et al. 1993)
4.50 (guppy, lipid normalized BCF, Sijm et al. 1993)
2.99 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption, Koelmans et al. 1993)
2.90, 3.28; 3.08, 3.41 (*Poecilla reticulata; Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
2.94–3.23 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
3.08, 4.16; 2.812, 3.055 (quoted: whole fish, lipid content; calculated- MCI χ, K_{OW}, Lu et al. 1999)
3.68; 3.72 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
2.85 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
2.73–4.00 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
4.70; 4.10 (field data of Lake Ontario sediment trap material; Niagara River-organic matter, Oliver & Charlton 1984)
3.0, 2.0 (Sanhedron soil humic acid, Suwannee River humic acid, batch equilibrium-sorption isotherm, GC/ECD, Chiou et al. 1986)
2.3, 2.0 (Sanhedron soil fulvic acid, Suwannee River fulvic acid, batch equilibrium-sorption isotherm, GC/ECD, Chiou et al. 1986)
3.21, 3, 14 (Riddles soil: top layer 1.84% OC; below top layer, batch equilibrium-sorption isotherm, Boyd et al. 1990)
3.18, 3.38, 3.43, 3.26, 3.23 (five soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
3.91 (Isora soil 1.87% OC, batch equilibrium, GC, Paya-Perez et al. 1991)
3.81 (lake sediment 2.5% OC, batch equilibrium, Schrap et al. 1994)
3.61 ± 0.39 (suspended particulates in coastal waters, Masunaga et al. 1996)
3.16 (HPLC-screening method; Müller & Kördel 1996)
3.48, 3.37 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environment Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} \sim 1.0 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹, residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)
k(aq.) ≤ 0.06 M^{-1} s^{-1} for direct reaction with ozone in water at pH 3 and 21°C, with $t_{½} > 6$ d at pH 7 (Yao & Haag 1991).
$k_{HO\cdot}$(calc) = 4.0×10^9 $M^{-1}s^{-1}$ in aqueous solutions (Haag & Yao 1992)
Hydrolysis: base rate constant k < 0.9 M^{-1} h^{-1} at 25°C with a calculated $t_{½} > 900$ yr at pH 7 (Ellington et al. 1988)
Biodegradation: dechlorination pseudo-first order rate constant k = 0.387 d^{-1} with $t_{½} = 1.8$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:
$k_1 = 8300$ d^{-1}; $k_2 = 0.45$ d^{-1} (guppy, exptl., Könemann & van Leeuwen 1980)
$k_2 = 0.45$ d^{-1} (guppy, exptl., Könemann & van Leeuwen 1980)

k_1 = 18.7 h^{-1}; $1/k_2$ = 53 h (guppy, quoted, Hawker & Connell 1985)
log k_1 = 2.50 d^{-1}; log k_2 = –0.35 d^{-1} (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)
k_1 = 780 mL $g^{-1}\cdot d^{-1}$; k_2 = 0.42 d^{-1} (guppy, Van Hoogan & Opperhuizen 1988)
k_1 = 780 ± 220 L kg^{-1} d^{-1}; k_2 = 0.42 ± 0.06 d^{-1} (guppy, 96-h exposure studies, Sijm et al. 1993)
k_1 = (23–29) mL g^{-1} d^{-1}, k_2 = (5–3) d^{-1} (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in one day or 12 sunlit hour at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)
Surface Water: $t_{½}$ = 1.9–30 d, surface waters in various locations in the Netherlands in case of first order reduction process may be assumed (estimated, Zoeteman et al. 1980)
hydrolysis $t_{½}$ > 900 yr at pH 7 and 25°C (Ellington et al. 1988)
k(exptl) ≤ 0.006 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21°C, with $t_{½}$ > 6 d at pH 7 (Yao & Haag 1991)
Groundwater:
Sediment: dechlorination $t_{½}$ = 1.8 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Soil:
Biota: biological $t_{½}$ < 1 d in trout, $t_{½}$ = 2 d in sunfish and $t_{½}$ = 2 d in guppy for trichlorobenzenes (Niimi 1987)
$t_{½}$ < 5 d in worm at 8°C (Oliver 1987a).

TABLE 6.1.1.5.1
Reported aqueous solubilities, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,3-trichlorobenzene at various temperatures

Aqueous solubility		log K_{OW}		log K_{OA}	
Shiu et al. 1997		Finizio & Di Guardo 2001		Harner & Mackay 1995	
shake flask-GC		GC-RT correlation		generator column-GC/ECD	
t/°C	S/g·m^{-3}	t/°C	log K_{OW}	t/°C	log K_{OA}
5	7.66	5	3.91	25	5.19
25	19.31	15	3.84	–10	6.491
50	45.61	25	3.81	0	6.073
		35	2.64	9.88	5.699
				19.85	5.829
				ΔH_{OA}/(kJ mol^{-1}) = 55.7	
				log K_{OA} = A + B/T	
				A	–4.6
				B	2909

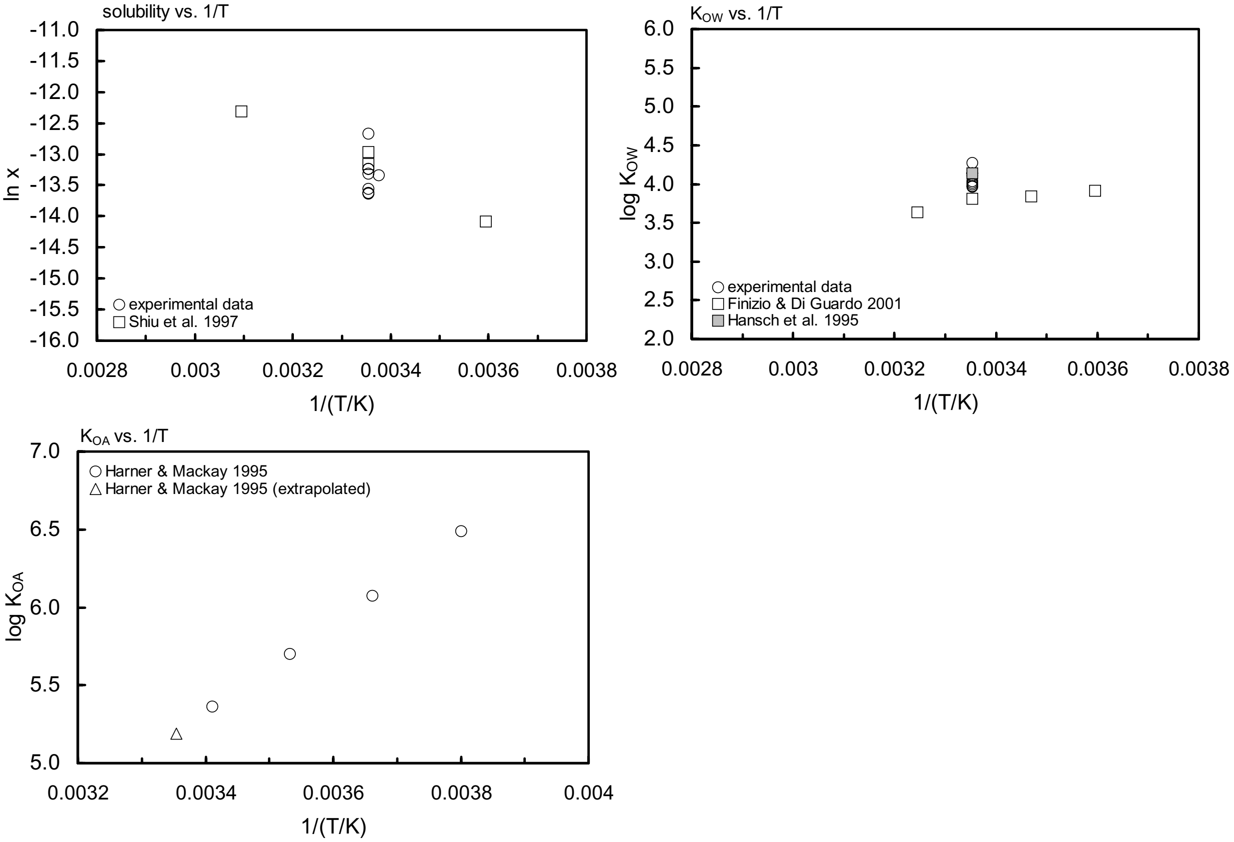


FIGURE 6.1.1.5.1 Logarithm of mole fraction solubility, K_{OW} and K_{OA} versus reciprocal temperature for 1,2,3-trichlorobenzene.

TABLE 6.1.1.5.2
Reported vapor pressures of 1,2,3-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln (P/P_o) = (1 - T/T_o) \cdot \exp[\Sigma A_i T^i]$ (5) - Cox eq.

$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)
$\ln P = A - B/(C + T/K)$ (3a)

1.

Stull 1947

summary of lit. data

t/°C	P/Pa
40	133.3
70	666.6
85.5	1333
101.8	2666
119.8	5333
131.5	7999
146.0	13332
168.2	26664
193.5	53329
218.5	101325
mp/°C	52.5

Sears & Hopke 1949

Rodebush gauge

t/°C	P/Pa
measure range: 16–30°C	
mp/°C	52.55 to 52.70
eq. 1	P/micron
A	13.662
B	3440.2

Liu & Dickhut 1994

gas saturation-GC

t/°C	P/Pa
–15	0.124
5.0	0.445
10	2.80
25	11.2
40	50.5

ΔH_V/(kJ mol^{-1}) = 54.5
(–15 to 40°C)

for solid
ΔH_{subl}/(kJ mol^{-1}) = 72.7

Polednicek et al. 1996

static method-pressure gauge

t/°C	P/Pa	t/°C	P/Pa
	solid		liquid
0.36	0.94	60.11	268.14
0.38	0.955	70.04	472.25
10.35	2.971	80.01	789.67
10.36	2.965	80.01	799.36
20.35	8.820	88.72	1241.7
20.37	8.834	88.73	1238.8
30.28	23.62	92.95	1305.6
30.28	23.66	98.72	1995.1
50.12	146.0	108.67	3055.0
50.12	145.5	118.69	4618.2
25	14.07	128.73	6805.3
	interpolated	138.77	9800.6
		138.78	9788.7
	solid	148.88	13815
eq. 3a	P/Pa	158.88	19090
A	33.2977	168.95	25970
B	9327.37		
C	6.13455		
			liquid
		eq. 3a	P/Pa
		A	21.1681
		B	4077.21
		C	–71.5639

2.

Roháč et al. 1999

recommended

T/K	P/Pa	T/K	P/Pa
	solid		liquid
233.15	0.003	333.15	272.4
243.15	0.015	343.25	479.4
253.15	0.065	353.15	812.0

(Continued)

TABLE 6.1.1.5.2 (*Continued*)

Roháč et al. 1999			
recommended			
T/K	P/Pa	T/K	P/Pa
263.15	0.26	363.15	1329
273.15	0.90	373.15	2106
283.15	2.90	383.15	3245
283.15	8.50	393.15	4868
303.15	23.1	403.15	7130
313.15	58.9	413.15	10220
323.15	140.9	423.15	14340
		433.15	19760
Data fitted to Cox eq.		443.15	26760
For solid		453.15	35700
eq. 5	P/Pa	463.15	46860
A_0	3.380608	473.15	6730
$10^{-4}A_1$	–2.5802866	483.15	77730
A_2	0	493.15	98350
T_o/K	325.6	503.15	123100
P_o/Pa	173.0		
bp/K	494.45	Cox eq.	
temp range 273–323 K		eq. 5	P/Pa
		A_0	3.274398
		$10^{-3}A_1$	–1.0923018
		$10^{-7}A_2$	7.8603029
		T_o/K	325.6
		P_o/Pa	173.0
		bp/K	494.45
		temp range 333–448 K	

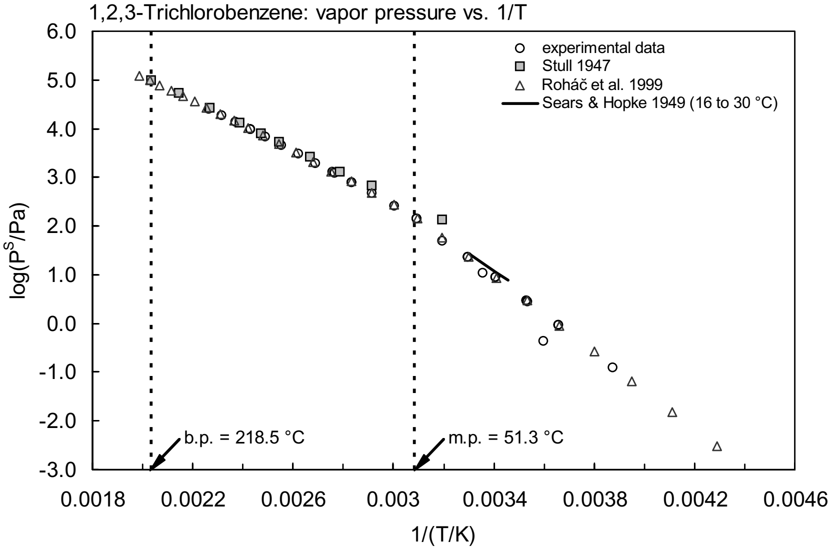
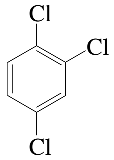


FIGURE 6.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3-trichlorobenzene.

6.1.1.6 1,2,4-Trichlorobenzene



Common Name: 1,2,4-Trichlorobenzene
Synonym: unsym-trichlorobenzene
Chemical Name: 1,2,4-trichlorobenzene
CAS Registry No: 120-82-1
Molecular Formula: $C_6H_3Cl_3$
Molecular Weight: 181.447
Melting Point (°C):
16.92 (Lide 2003)
Boiling Point (°C):
213.5 (Weast 1972–73; Lide 2003)
Density (g/cm^3 at 20°C):
1.4542 (Weast 1972–73)
1.446 (Dean 1985, 1992)
1.459 (Lide 2003)
Molar Volume (cm^3/mol):
124.8 (20°C, calculated-density)
158.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
15.48 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.56 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio, at 25°C, F: 1.0 (Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
25.03 (Irmann 1965)
34.7 (shake flask-UV, Yalkowsky et al. 1979)
30.0 (Callahan et al. 1979)
19.4 (shake flask-GC, Könemann 1981)
30.0 (recommended, Hovarth 1982)
48.8 (20°C, shake flask-GC, Chiou & Schmedding 1981; Chiou et al. 1982; 1983)
46.1 (generator column-GC/ECD, Miller et al. 1984; 1985)
31.3 (shake flask-HPLC/UV, Banerjee 1984)
30.9 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
34.6 (shake flask-GC, Chiou 1985)
52.0 (shake flask-GC, Boyd et al. 1998)
36.5* ± 0.36 (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)
7.71, 10.39, 13.58, 19.82 (5, 15, 25, 35°C, estimated- RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (38.4°C, summary of literature data, temp range 38.4–213°C, Stull 1947)
38.6 (calculated by formula, Dreisbach 1955)
$\log (P/mmHg) = 7.19608 - 1827.0/(210.0 + t/°C)$; temp range 110–280°C (Antoine eq. for liquid state, Dreisbach 1955)
60.6 (extrapolated-Antoine eq., supercooled liquid, Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 11425.1/(T/K)] + 8.030523$; temp range 38.4–213°C (Antoine eq., Weast 1972–73)

26.4 (gas saturation, Politzki et al. 1982)
28.5 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
38.7 (interpolated-Antoine eq-III, Stephenson & Malanowski 1987)
$\log (P_S/\text{kPa}) = 9.570 - 3254/(T/K)$; temp range 279–290 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.31998 - 1827/(-63.15 + T/K)$; temp range 383–553 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.6802 - 2064.4/(-43.05 + T/K)$; temp range 293–383 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
53.4 (supercooled liquid P_L, GC-Kovás retention indices correlation; Spieksma et al. 1994)
$\log (P/\text{mmHg}) = 15.5947 - 2.8920 \times 10^3/(T/K) - 2.5549 \cdot \log (T/K) + 2.0384 \times 10^{-4} \cdot (T/K) - 7.0601 \times 10^{-14} \cdot (T/K)^2$, temp range 290–725 K, (Yaws 1994)
5728* (118.671°C, comparative ebulliometry, measured range 118.671–215.887°C, Roháč et al. 1998)
24.2* (20°C, recommended, summary of literature data, temp range 293.15–493.15 K, Roháč et al. 1999)
$\ln [(P/\text{Pa})/19.0] = [1 - (T/K)/290.07] \cdot \exp\{3.352607 - 9.0343639 \times 10^{-4} \cdot (T/K) + 6.0501757 \times 10^{-7} (T/K)^2\}$; temp range 294–489 K (Cox eq., recommended, Roháč et al. 1999)
$\log (P/\text{kPa}) = 9.570 - 3254/(T/K)$; temp range 6–17°C (solid, regression eq. from literature data, Shiu & Ma 2000)
$\log (P/\text{kPa}) = 6.682 - 2064.4/[(T/K) - 43.5]$; temp range 20–110°C (liquid, regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

122 (gas stripping-GC, Oliver 1985)
144 (gas stripping-GC, Warner et al. 1987)
195* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
$\ln [H/(\text{atm} \cdot m^3/\text{mol})] = -16.34 + 3307/(T/K)$; temp range 10–30°C (EPICS-GC/FID, Ashworth et al. 1988)
101 (gas stripping-GC, ten Hulscher et al. 1992)
375.2 (modified EPICS method-GC, Ryu & Park 1999)
172 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 4.381 - 1622/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.05 (Leo et al. 1971)
4.26 (Callahan et al. 1979)
4.02 (Hansch & Leo 1979; Hansch & Leo 1985)
3.93 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
4.02 (20°C, shake flask-GC, Chiou & Schmedding 1981; Chiou et al. 1982; Chiou 1985)
3.97 (shake flask-GC, Watarai et al. 1982)
3.96 (HPLC-k′ correlation, Hammers et al. 1982)
3.93–4.18, 4.09 (range, mean, shake flask method, Eadsforth & Moser 1983)
4.12–4.32, 4.21 (range, mean, HPLC method, Eadsforth & Moser 1983)
3.98 (generator column-GC/ECD, Miller et al. 1984; 1985)
4.22 (HPLC-k′ correlation, De Kock & Lord 1987)
4.02 (shake flask-GC, Pereira et al. 1988)
4.05 (slow stirring-GC, De Bruijn et al. 1989)
4.02 (recommended, Sangster 1993)
4.02 (recommended, Hansch et al. 1995)
3.92* (estimated- RP-HPLC-k′ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.

5.10* (20°C, HPLC-k′ correlation, measured range 10–50°C, Su et al. 2002)
$\log K_{OA} = 62080/(2.303 \cdot RT) - 6.031$; temp range 10–50°C (HPLC-k′ correlation, Su et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:
3.32 (fathead minnow, 32-d exposure, Veith et al. 1979b)
3.45; 3.37; 2.95 (fathead minnow; green sunfish; rainbow trout, Veith et al. 1979b)
2.69 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980a)
2.26 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
3.52 (microorganism-water, Mabey et al. 1982)
3.04–3.11 mean 3.11; 3.43–3.60 mean 3.51 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
4.19–4.56 (rainbow trout, lipid base, Oliver & Niimi 1983)
3.26–3.61 (fish, Oliver 1984, 1985)
2.40 (algae, Geyer et al. 1984)
3.15 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
2.40, 2.69, 3.15 (algae, fish, sludge, Klein et al. 1984)
3.15–3.72 mean 3.36; 3.30–3.75 mean 3.57 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)
3.11; 3.08 (rainbow trout, wet wt. basis, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)
4.19–4.56 (rainbow trout, lipid base, Oliver & Niimi 1985)
2.09; 3.84 (quoted, rainbow trout, 1.8% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
2.28, 2.40, 2.34, 2.66 (quoted, carp, 2.2% lipid, wet wt basis, Geyer et al. 1985)
3.94, 3.96, 4.0, 4.32 (quoted, carp, 2.2% lipid, lipid basis, Geyer et al. 1985)
2.54; 4.04 (quoted, rainbow trout, hatching, 3.2% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
2.66, 2.73; 4.02, 4.09 (quoted, carp, 4.4% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
2.96; 4.26 (quoted, golden ide, 5.0% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
2.86, 2.94; 4.15, 4.19 (quoted, zebra fish, 5.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
2.83, 3.12; 4.12, 4.22 (quoted, tilapia, 5.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
2.98, 3.12; 4.23, 4.36 (quoted, bluegill sunfish, 5.7% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
3.13, 3.14; 4.37, 4.38 (quoted, guppy, 5.8% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
3.11, 3.20; 4.23, 4.38 (quoted, rainbow trout, 7.7%, wet wt basis; lipid basis, Geyer et al. 1985)
2.96, 3.03; 4.05, 4.23 (quoted, guppy, 8.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
3.11; 4.19 (quoted, rainbow trout, 8.3% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
3.32; 4.30 (quoted, fathead minnow, 10.5% lipid, wet wt basis, lipid basis Geyer et al. 1985)
2.69; 2.40; 3.15 (fish; algae; activated sludge, Freitag et al. 1985)
2.61 (fathead minnow, Carlson & Kosian 1987)
4.76, 4.90, 3.54, 4.68 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.31, 4.25 (American flagfish, whole fish, fish lipid, Smith et al. 1990)
2.95–3.57; 3.31; 3.32; 3.36 (*Oncorhynchus mykiss; Jordanella floridae; Pimephales promelas; Lepomis cyanellus*, quoted lit., flow through conditions, Devillers et al. 1996)
3.0, 3.06, 3.06 (guppy: k_1/k_2-best fit exptl. data, k_1/k_2-slope method, C_f/C_w-steady state, van Eck et al. 1997)
3.81; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
2.80 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
2.68–3.94 (5 soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
4.70; 4.40 (field data of sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
4.3–5.1, 5.10; 5.10 (suspended sediment, average; algae > 50 μm, Oliver 1987c)
4.8–5.3, 5.0 (Niagara River plume, range, mean, Oliver 1987b)
3.91 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.66, 3.40 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.27 (untreated Marlette soil B_t horizon, 0.30% OC, equilibrium isotherm, Lee et al. 1989)

3.91, 3.64, 3.04 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.32 (calculated-K_{OW}, Aldrich or Fluka humic acid polymers, Chin & Weber 1989)
3.32; 2.62 (Aldrich humic acid, organic polymers, Chin et al. 1990)
4.02 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
2.71, 2.71 (RP-HPLC-k′ correlation including: MCI-related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
3.86 ± 0.40 (suspended particulates in coastal waters, Masunaga et al. 1996)
3.15, 3.19, 3.10 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
4.38–3.24 (NIST SRM diesel particulate matter, sorption isotherm, Ngyuen et al. 2004)

Sorption Partition Coefficient, log K_{OM}:
2.70 (Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm, Chiou et al. 1983)
2.89 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.47, 3.17 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.97 (untreated Marlette soil B_t horizon, 0.30% OC, equilibrium sorption isotherm, Lee et al. 1989)
3.97, 3.50, 2.87 (organic cations treated Marlette soil B_t horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k or Half-Lives. $t_{½}$:
Volatilization: rate constants: $k = 0.032\ d^{-1}$ with $t_{½} = 22$ d in spring at 8–16°C, $k = 0.066\ d^{-1}$ with $t_{½} = 11$ d in summer at 20–22°C, $k = 0.058\ d^{-1}$ with $t_{½} = 12$ d in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.073\ d^{-1}$ with $t_{½} = 9.5$ d with $HgCl_2$, and $k = 0.066\ d^{-1}$ with $t_{½} = 10.6$ d without $HgCl_2$ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)
Photolysis: not environmentally relevant (Mabey et al. 1982)
$t_{½} = 450$ yr for surface water photolysis at 40°N latitude in the summer (Dulin et al. 1986)
$k = 1.16 \times 10^{-3}\ h^{-1}$ with H_2O_2 at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988)
$k = 0.03\ h^{-1}$, the maximum summer photolysis rate calculated at midday clear sky, the minimum photolytic $t_{½} \sim 4$ months, but a realistic value is likely to be at least 1 yr (Bunce et al. 1989)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k = 7.22 \times 10^{-3}\ h^{-1}$ (Simmons et al. 1976; selected, Mackay et al. 1985)
$k_{OH} \sim 1.0 \times 10^{-13}\ cm^3\ molecule^{-1}\ s^{-1}$, residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)
k(singlet oxygen) << 360 $M^{-1}\ h^{-1}$; k (RO_2 radical) << 1 $M^{-1}\ h^{-1}$ (Mabey et al. 1982)
k << 1.6 $M^{-1}\ s^{-1}$ for the reaction with ozone in water using 10 mM *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)
$k_{OH} = 5.32 \times 10^{-13}\ cm^3\ molecule^{-1}\ s^{-1}$ at 296 K, measured range 273–368 K (flash photolysis-resonance fluorescence, Rinke & Zetzsch 1984)
k_{OH} (obs.) = $5.32 \times 10^{-13}\ cm^3\ molecule^{-1}\ s^{-1}$; and k_{OH}(calc) = $3.47 \times 10^{-13}\ cm^3\ molecule^{-1}\ s^{-1}$ at room temp. (Atkinson 1985)
k_{OH}(calc) = $0.29 \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$, k_{OH}(obs) = $0.532 \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_{OH}(aq.) = $4.0 \times 10^9\ M^{-1}s^{-1}$ in aqueous solutions (Haag & Yao 1992)
k_{OH}(calc) = $0.34 \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis: not environmentally significant (Mabey et al. 1982);
base rate constant $k < 0.9\ M^{-1}\ h^{-1}$ at 25°C with a calculated $t_{½} > 900$ yr at pH 7 (Ellington et al. 1988)
first-order rate constant $k = 2.3 \times 10^{-5}\ h^{-1}$ with $t_{½} = 3.4$ yr at pH 7 and 25°C (Howard et al. 1991).
Biodegradation: $k = 1.92 \times 10^{-2}\ h^{-1}$, degradation in water (Simmons et al. 1976)
$t_{½}$(aq. aerobic) = 672–4320 h estimated from unacclimated soil grab sample data (Howard et al. 1991)
$t_{½}$(aq. anaerobic) = 2688–17280 h based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

k = 0.05 d^{-1}, significant degradation in an aerobic environment (Tabak et al. 1981; Mills 1982)
k = 0.029 d^{-1} in river water, k = 0.026 d^{-1} in estuarine water, and k = 0.012 d^{-1} in marine water (Bartholomew & Pfaender 1983; Battersby 1990)
$t_{½}$(aerobic) = 28 d, $t_{½}$(anaerobic) = 110 d in natural waters (Capel & Larson 1995)
k = 0.035 d^{-1}, the dechlorination pseudo-first order rate constant, with $t_{½}$ =19.8 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000)

Biotransformation: 1×10^{-10} mL $cell^{-1}$ h^{-1} (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 8300 d^{-1}; k_2 = 0.45 d^{-1} (guppy, exptl., Könemann & Van Leeuwen 1980)
k_1 = 18.7 h^{-1}; $1/k_2$ = 53.0 h (guppy, selected, Hawker & Connell 1985)
log k_1 = 2.65 d^{-1}; log $1/k_2$ = 0.34 d (guppy, selected, Connell & Hawker 1988)
log k_2 = –1.85 d^{-1}; log k_2 = 0.23 d^{-1} (fish, calculated-K_{OW}, fast-biphasic, Thomann 1989)
k_1 = 1158 d^{-1}, 10140 d^{-1}; k_2 = 0.57 d^{-1}, 0.57 d^{-1} (American flagfish: whole fish, fish lipid, Smith et al. 1990)
k_2 = 0.57 d^{-1}, 0.46 d^{-1} (American flagfish: bioconcentration data, toxicity data, Smith et al. 1990)
k_1 = 492 ± 234 L kg^{-1} d^{-1}; k_2 = 0.49 ± 0.22 d^{-1} (guppy, exptl., van Eck et al. 1997)

Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in one day or 12 sunlit hour at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)
calculated minimum photolytic $t_{½}$ ~4 months, but realistically at least 1 yr (Bunce et al. 1989);
tropospheric lifetime of 25 d based on reaction principally with OH radical and other photochemical reactions (Bunce 1991);
$t_{½}$ = 128.4–1284 h, based on the photooxidation with OH radical (Howard et al. 1991).

Surface Water: $t_{½}$ = 2.1–28 d estimated for various locations in the Netherlands, $t_{½}$ = 0.3–3 d for river water, $t_{½}$ = 3–30 d for lakes estimated from persistence (Zoeteman et al. 1980);
half-lives from marine mesocosm: $t_{½}$ = 22 d in the spring at 8–16°C, $t_{½}$ = 11 d in the summer at 20–22°C and $t_{½}$ = 12 d in the winter at 3–7°C when volatilization dominates, and $t_{½}$ = 9.5 d and 10.6 d for experiments with and without $HgCl_2$ respectively in September 9–15 (Wakeham et al. 1983)
hydrolysis $t_{½}$ > 900 yr at pH 7 and 25°C (Ellington et al. 1988)
$t_{½}$(aerobic) = 672–4320 h, based on unacclimated aerobic soil grab sample data; $t_{½}$(anaerobic) = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life; and first order hydrolysis $t_{½}$ = 3.4 yr (Howard et al. 1991);
$t_{½}$(aerobic) = 28 d, $t_{½}$(anaerobic) = 110 d in natural waters (Capel & Larson 1995)

Groundwater: $t_{½}$ = 1344–8640 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
$t_{½}$ = 30–300 d estimated from persistence (Zoeteman et al. 1980).

Soil: $t_{½}$ < 10 d (Ryan et al. 1988)
$t_{½}$ = 672–4320 h, based on unacclimated aerobic soil grab sample data (Howard et al. 1991).

Sediment: dechlorination $t_{½}$ = 19.8 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biota: 1 < $t_{½}$ < 3 d in blue bluegill sunfish (Barrows et al. 1980);
biological half-lives, $t_{½}$ < 1 d in trout, $t_{½}$ = 2 d in sunfish, and $t_{½}$ = 2 d in guppy for trichlorobenzenes (Niimi 1987);
$t_{½}$ < 5 d in worms at 8°C (Oliver 1987a);
depuration $t_{½}$ = 1.21 d from whole fish, $t_{½}$ = 1.20 d from fish lipid (American flagfish, Smith et al. 1990).

TABLE 6.1.1.6.1
Reported aqueous solubilities of 1,2,4-trichlorobenzene at various temperatures

Ma et al. 2001		Finizio & Di Guardo 2001	
shake flask-GC		RP-HPLC-k′ correlation	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
5	32.9	5	7.71
15	28.5	15	10.39
25	36.5	25	13.58
35	39.8	35	19.82
45	46.5		

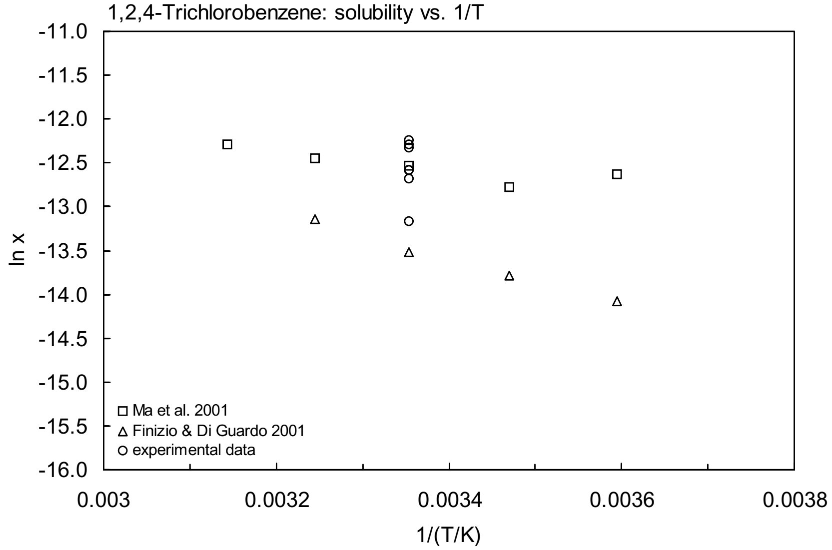


FIGURE 6.1.1.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,2,4-trichlorobenzene.

TABLE 6.1.1.6.2
Reported vapor pressures of 1,2,4-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln (P/P_o) = (1 - T/T_o) \cdot \exp[\Sigma A_i T^i]$ (5) - Cox eq.
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)
$\ln P = A - B/(C + T/K)$ (3a)

Stull 1947		Sears & Hopke 1949		Roháč et al. 1998		Roháč et al. 1999	
summary of literature data		Rodebush gauge		comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
38.4	133.3	measured range: 6–25°C		118.671	5728	293.15	24.2
67.3	666.6			128.383	8331	303.15	51.2
81.7	1333	mp/°C	17.05–17.40	136.228	11070	313.15	102.4
97.2	2666			142.813	13911	232.15	194.7
114.8	5333	for solid:-		142.819	13914	333.15	354.0
125.7	7999	eq. 1	P/micron	148.44	16794	343.25	617.7
140	13332	A	13.445	154.289	20281	353.15	1038
162	26664	B	3254.0	154.308	20290	363.15	1687
187.7	53329			160.441	24566	373.15	2658
213	101325	for liquid:-		166.386	29387	383.15	4071
		eq. 1	P/micron	172.180	34807	393.15	6075
mp/°C	17.0	A	10.682	177.755	40745	403.15	8854
		B	2452.3	183.424	47613	413.15	12630
				192.328	60271	423.15	17650
				192.331	60264	433.15	224210
				200.386	74748	443.15	32650
				209.989	93380	453.15	43360
				212.397	98847	463.15	56740
				215.887	107216	473.15	73260
						483.15	93420
				bp/°C	213.492	493.15	117800
				eq. 3	P/kPa	eq. 5	P/Pa
				A	6.11973	A_0	3.352607
				B	1677.35	$10^{-3}A_1$	–9.0343639
				C	–78.926	$10^{-7}A_2$	6.0501757
						T_o/K	290.07
						P_o/Pa	19.0
						bp/K	486.60
						temp range 294–489 K	

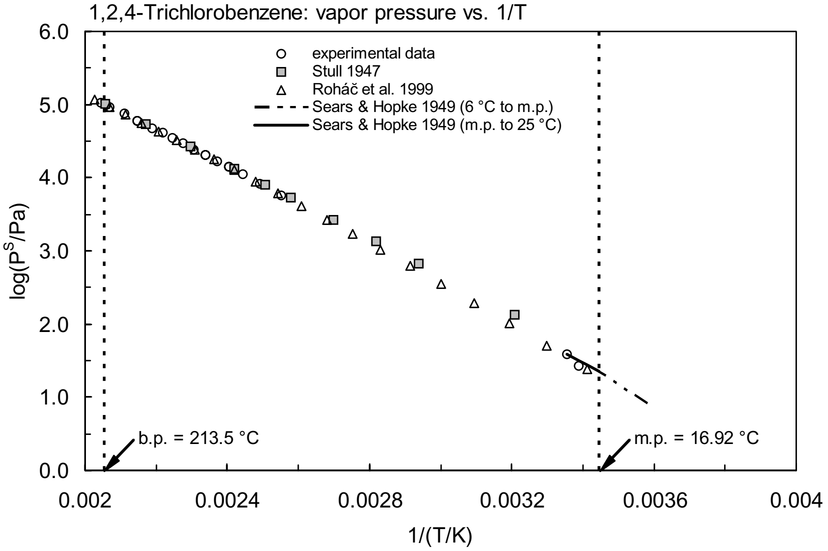


FIGURE 6.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4-trichlorobenzene.

TABLE 6.1.1.6.3
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,4-trichlorobenzene at various temperatures

Henry's law constant		log K_{OW}		log K_{OA}	
Ashworth et al. 1988		Finizio & Di Guardo 2001		Su et al. 2002	
EPICS-GC		HPLC-RT correlation		GC-RT correlation	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OW}	t/°C	log K_{OA}
10	131	5	4.12	10	5.45
15	106	15	4.02	20	5.1
20	185	25	3.92	30	4.77
20	195	35	3.8	40	4.46
30	301			50	4.17
ln (H/(atm m³/mol) = A – B/(T/K)				ΔH_{OA}/(kJ mol⁻¹) = 62.08	
A	7.261				
B	4028			log K_{OA} = A + B/2.303RT	
				A	–6.031
				B	62080

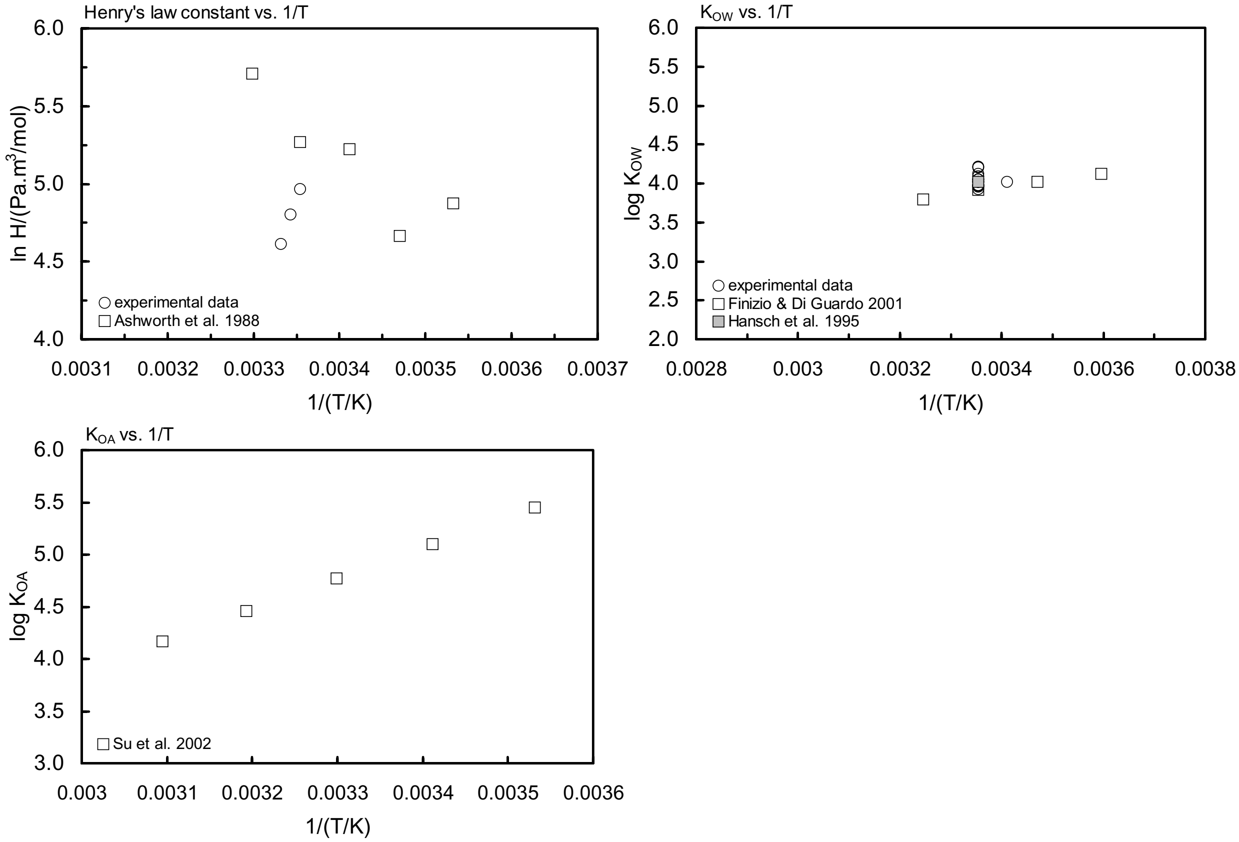
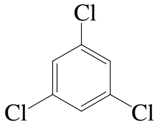


FIGURE 6.1.1.6.3 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for 1,2,4-trichlorobenzene.

6.1.1.7 1,3,5-Trichlorobenzene



Common Name: 1,3,5-Trichlorobenzene
Synonym: sym-trichlorobenzene
Chemical Name: 1,3,5-trichlorobenzene
CAS Registry No: 108-70-3
Molecular Formula: $C_6H_3Cl_3$
Molecular Weight: 181.447
Melting Point (°C):
  62.8 (Lide 2003)
Boiling Point (°C):
  208.0 (Weast 1972–72, 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
  1.3865 (64°C, Weast 1972–73; Horvath 1982)
Molar Volume (cm^3/mol):
  130.9 (64°C, calculated-density)
  125 (calculated-density, liquid molar volume, Chiou 1985)
  158.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  19.622 (Tsonopoulos & Prausnitz 1971)
  18.786 (Miller et al. 1984)
  18.198 (Ruelle et al. 1993; Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  58.16 (Tsonopoulos & Prausnitz 1971)
  56.07 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.426 (mp at 62.8°C)
  0.413 (25°C, Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  25.03 (Tsonopoulos & Prausnitz 1971)
  6.59 (shake flask-UV, Yalkowsky et al. 1979)
  5.87 (shake flask-GC, Könemann 1981)
  6.61 (recommended, Hovarth 1982)
  4.12 (generator column-GC/ECD, Miller et al. 1984, 1985)
  6.01 (shake flask-HPLC, Banerjee 1984)
  10.6 (shake flask-GC, Chiou 1985)
  6.53 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
  8.46* ± 0.26 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
  2.40 (shake flask-GC, Boyd et al. 1998)
  $\ln x = -5.083768 - 2650.68/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  666.6* (63.8°C, summary of literature data, temp range 63.8–208.4°C, Stull 1947)
  77 (extrapolated-Antoine eq., supercooled liquid, Weast 1972–73)
  $\log (P/mmHg) = [-0.2185 \times 11211.0/(T/K)] + 7.977218$; temp range 63.8–208.4°C (Antoine eq., Weast 1972–73)
  30.23 (gas saturation, interpolated from reported graph, Rordorf 1985)
  24.4 (solid, extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_S/kPa) = 8.301 – 2956/(T/K); temp range 282–301 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.43345 – 1932.26/(–45.268 + T/K); temp range 336–482 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
124.4 (GC-RT correlation, Watanabe & Tatsukawa 1989)
62.4; 74.9 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
log (P/mmHg) = 19.2854 – 4.4976 × 10^3/(T/K) – 3.6158·log (T/K) – 5.2495 × 10^{-9}·(T/K) + 1.5596 × 10^{-6}·$(T/K)^2$, temp range 398–748 K (Yaws 1994)
12.4, 20.44* (20.35°C pressure gauge measurement, 25°C interpolated from reported Antoine eq. based on exptl. data, Polednicek et al. 1996)
ln (P_S/Pa) = 32.5109 – 8909.70/[(T/K) + 3.94116]; temp range 273–333 K (Antoine eq. from exptl data, pressure gauge measurement, solid, Polednicek et al. 1996)
ln (P_L/Pa) = 21.1215 – 3939.96/[(T/K) – 71.2907]; temp range 343–442 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Polednicek et al. 1996)
12.5 (20°C, recommended, summary of literature data, temp range 233.15–483.15 K, Roháč et al. 1999)
ln [(P_S/Pa)/565.0] = [1 – (T/K)/337.0)·exp{3.305508 – 2.3049477 × 10^{-4}·(T/K)}; temp range 273–333 K (Cox eq., solid, recommended, Roháč et al. 1999)
ln [(P_L/Pa)/547.0] = [1 – (T/K)/336.6)·exp{3.190854 – 1.0710853 × 10^{-3}·(T/K) + 7.5659237 × $10^{-7}$$(T/K)^2$}; temp range 343–442 K (Cox eq., liquid, recommended, Roháč et al. 1999)
32.3* (29.33°C, static method-diaphragm manometer, measured range 29–142°C, Blok et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
192.5 (20°C, batch stripping-GC, Oliver 1985)
192 (gas stripping-GC/ECD, ten Hulscher et al. 1992)

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
4.02 (Leo et al. 1971; Hansch & Leo 1979)
4.15 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
4.17 (shake flask-GC, Watarai et al. 1982)
4.17 (HPLC-k′ correlation, Hammers et al. 1982)
4.02 (generator column-GC/ECD, Miller et al. 1984; 1985)
4.18 (HPLC-RV correlation, Garst 1984)
4.31 (shake flask-GC, Chiou 1985)
4.49 (Hansch & Leo 1985)
4.32* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)
4.31 (shake flask-GC, Pereira et al. 1988)
4.189 (slow stirring-GC, De Bruijn et al. 1989)
4.15 (recommended, Sangster 1993)
4.19 (recommended, Hansch et al. 1995)
4.34* ± 0.04 (shake flask-GC/ECD, Bahadur et al. 1997)
log K_{OW} = 1.1228 – 18200/[2.303·R(T/K)]; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
4.44 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
4.85 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)
4.89* (20°C HPLC-k′ correlation, measured range 10–50°C, Su et al. 2002)
log K_{OA} = 68550/(2.303·RT) – 7.368; temp range 10–50°C (HPLC-k′ correlation, Su et al. 2002)

Bioconcentration Factor, log BCF: at 25°C or as indicated
4.15 (guppy, lipid basis, Könemann & van Leeuwen 1980)
3.15–3.30 mean 3.26; 3.57–3.92 mean 3.61 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
4.34–4.67 (rainbow trout, lipid basis, Oliver & Niimi 1983)
3.26–3.61 (fish, Oliver 1984)

4.15 (guppy, female, 5.4% lipid, wet wt basis; lipid basis, Geyer et al. 1985)

2.39–2.55 (fish, normalized, Tadokoro & Tomita 1987)

4.14 (guppy-lipid phase, Gobas et al. 1987, 1989)

2.88 (fish, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)

4.32, 4.35, 4.38, 4.43 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)

4.40, 4.45, 3.51, 4.22 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)

3.26, 3.61; 3.48 (*Oncorhynchus mykiss; Poecilia reticula*, quoted lit., flow through conditions, Devillers et al. 1996)

2.68 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)

3.26, 4.33; 3.271, 2.884 (quoted: whole fish, lipid content; calculated-MCI χ, K_{OW}, Lu et al. 1999)

3.69; 3.64 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

5.10; 4.20 (field data of Lake Ontario sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)

2.85 (forest soil 0.2% OC, observed, Seip et al. 1986)

4.13 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)

3.55 ± 0.47 (suspended particulates in coastal waters, Masunaga et al. 1996)

3.69 (soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 4.5 h from a model river of 1 m depth with water current 1 m/s and wind velocity 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: may be susceptible to direct photolysis by sunlight (Howard 1989)

$t_{1/2}$ ~450 yr for sunlight photolysis at 40°N in the summer (Dulin et al. 1986)

$k = 0.003\ \text{min}^{-1}$, measured pseudo-first-order direct photolysis reaction with $t_{1/2} = (205.5 \pm 7.5)$ min in aqueous solution (Peijnenburg et al. 1992)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} \sim 1.0 \times 10^{-13}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$, residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

photooxidation $t_{1/2}$ = 6.17 months, based on a measured rate for the vapor phase reaction with photochemically produced hydroxyl radicals in air (Atkinson et al. 1985).

Hydrolysis: will not hydrolyze under normal environmental conditions (Howard 1989).

Biodegradation: resistant to biodegradation (Tabak et al. 1964; Howard 1989);

dechlorination pseudo-first order rate constant $k = 0.069\ \text{d}^{-1}$ with $t_{1/2}$ = 10.1 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 8000\ \text{d}^{-1}$; $k_2 = 0.40\ \text{d}^{-1}$ (guppy, Könemann & van Leeuwen 1980)

$k_1 = 18.0\ \text{h}^{-1}$; $1/k_2 = 60$ h (guppy, quoted, Hawker & Connell 1985)

$k_1 = 430\ \text{d}^{-1}$ (fish, quoted, Opperhuizen 1986)

$\log k_1 = 2.63\ \text{d}^{-1}$; $\log k_2 = 0.440\ \text{d}^{-1}$ (fish, quoted, Connell & Hawker 1988)

$\log k_1 = 2.48\ \text{d}^{-1}$; $\log k_2 = -0.40\ \text{d}^{-1}$ (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)

$\log k_2 = -0.40\ \text{d}^{-1}$ (fish, calculated-K_{OW}, Thomann 1989)

$k_1 = 7\ \text{mL g}^{-1}\ \text{d}^{-1}$, $k_2 = 3\ \text{d}^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in 1 d or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

Surface Water: $t_{1/2}$ = 18 d under field conditions in the Netherlands in case of first order reduction process may be assumed (estimated, Zoeteman et al. 1980)

direct photolysis $t_{1/2}$ = 206 min in aqueous solution (Peijnenburg et al. 1992)

Groundwater:.

Sediment: dechlorination $t_{1/2}$ = 1.8 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota: biological half-lives, $t_{1/2}$ < 1 d in trout, $t_{1/2}$ = 2 d in sunfish and $t_{1/2}$ = 2 d in guppy for trichlorobenzenes (Niimi 1987);

$t_{1/2}$ < 5 d in worms at 8°C (Oliver 1987a).

TABLE 6.1.1.7.1
Reported aqueous solubilities, octanol-water partition coefficients and octanol-air partition coefficients of 1,3,5-trichlorobenzene at various temperatures

Aqueous solubility		log K_{OW}				log K_{OA}	
Shiu et al. 1997		Opperhuizen et al. 1988		Bahadur et al. 1997		Su et al. 2002	
shake flask-GC		shake flask-GC/ECD		shake flask-GC/ECD		GC-RT correlation	
t/°C	S/g·m^{-3}	t/°C	log K_{OW}	t/°C	log K_{OW}	t/°C	log K_{OA}
5	4.62	13	4.40	5	4.52	25	5.23
15	6.29	19	4.32	15	4.43	–10	4.89
25	8.46	28	4.04	25	4.34	0	4.56
35	11.14	33	3.93	35	4.21	10	4.26
45	15.55			45	4.09	18.7	3.98
ΔH_{sol} = 22.04 kJ/mol		ΔH/(kJ mol^{-1}) = –21.7		enthalpy of transfer		ΔH_{OA}/(kJ mol^{-1}) = 68.55	
				ΔH/(kJ mol^{-1}) = –18.2			
				log K_{OW} = A – ΔH/2.303RT		log K_{OA} = A + B/2.303RT	
				A	1.1228	A	–7.368
				ΔH	–18200	B	68500

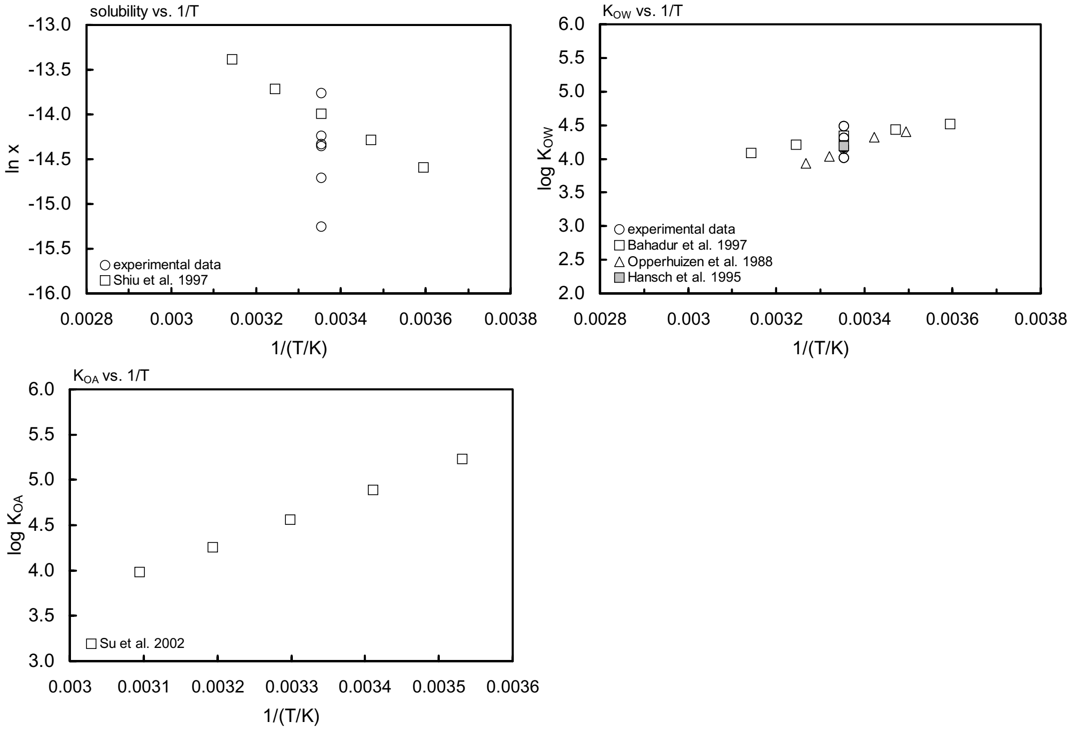


FIGURE 6.1.1.7.1 Logarithm of mole fraction solubility, K_{OW} and K_{OA} versus reciprocal temperature for 1,3,5-trichlorobenzene.

TABLE 6.1.1.7.2
Reported vapor pressures of 1,3,5-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3) $\ln P = A - B/(C + T/K)$ (3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

1.

Stull 1947		Sears & Hopke 1949		Polednicek et al. 1996			
summary of lit. data		Rodebush gauge		pressure gauge			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
					solid		liquid
63.8	666.6	measured between		0.29	1.493	70.04	760.47
78.0	1333	9–28°C	solid	0.29	1.383	70.05	759.77
93.7	2666			10.31	4.492	80.05	126.39
110.8	5333	eq. 1	P/μm	10.31	4.556	88.76	1956.9
121.8	7999	A	12.176	20.25	12.41	88.77	1954.0
136.0	13332	B	2956.0	20.25	12.40	89.95	2007.8
157.7	26664			30.15	34.58	90.01	2009.2
183.0	53329	mp/°C	63.45 to	30.15	34.56	99.25	3041.1
208.4	101325		63.50	40.09	83.96	108.75	4625.3
				40.09	83.89	118.8	6879.8
				50.09	193.4	128.8	9960.8
mp/°C	63.5			60.13	442.4	138.89	14257
				25	20.44	148.98	19754
					interpolated	159.03	27045
						169.13	36475
					solid	169.15	36355
				eq. 3a	P/Pa		
				A	32.5109		
				B	8909 70		liquid
				C	3.94116	eq. 3a	P/Pa
						A	21.1215
						B	3939.56
						C	–71.2907

2.

Blok et al. 2001					
torsion, mass-loss effusion		static-diaphragm manometer		static-diaphragm manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
	solid		solid	series I	liquid
–17.65	0.167	29.33	32.3	65.7	586
–15.65	0.218	29.34	32.3	68.1	669
–14.15	0.265	32.38	43.2	70.0	740
–12.15	0.343	32.38	43.6	72.17	828
–10.65	0.416	35.37	56.9	75.06	963
–9.15	0.502	38.38	74.0	77.84	1110
–7.15	0.643	38.39	74.4	79.57	1200

TABLE 6.1.1.7.2 *(Continued)*

Blok et al. 2001					
torsion, mass-loss effusion		**static-diaphragm manometer**		**static-diaphragm manometer**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
–5.15	0.822	41.43	95.4	81.90	1350
–3.65	0.984	44.47	122	83.47	1460
–0.65	1.40	47.57	157	series II	
		50.51	197	76.43	1050
		53.61	254	84.40	1550
		57.47	253	91.37	2140
		57.48	338	98.34	2920
		57.48	344	105.31	3940
		57.48	342	112.28	5230
		57.48	341	119.25	6880
		57.49	340	123.23	7990
				127.21	9240
				131.18	10600
		$\Delta H_{subl}/(kJ\ mol^{-1})$ = 70.74		135.16	12200
		at 298.15 K		139.14	13900
				142.12	15200
				$\Delta H_V/(kJ\ mol^{-1})$ = 50.27	
				at 375 K	

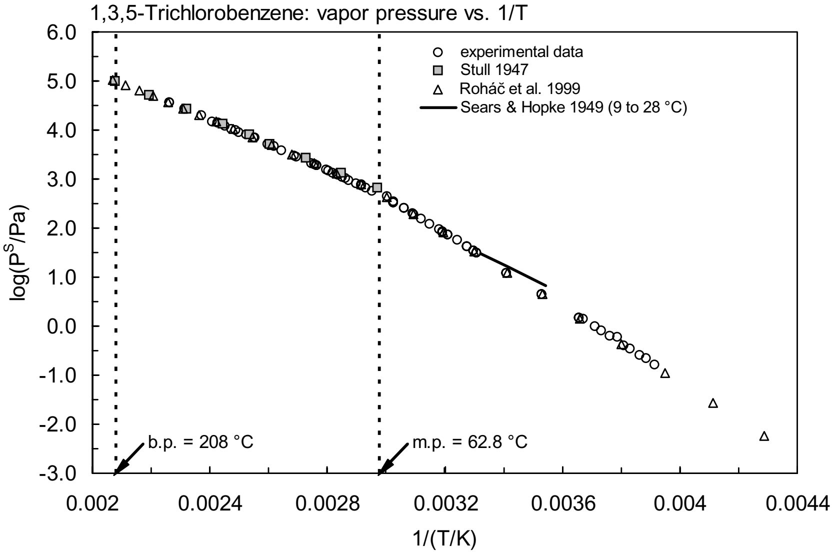
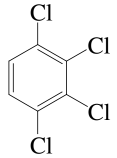


FIGURE 6.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trichlorobenzene.

6.1.1.8 1,2,3,4-Tetrachlorobenzene



Common Name: 1,2,3,4-Tetrachlorobenzene
Synonym:
Chemical Name: 1,2,3,4-tetrachlorobenzene
CAS Registry No: 634-66-2
Molecular Formula: $C_6H_2Cl_4$
Molecular Weight: 215.892
Melting Point (°C):
47.5 (Weast 1972–73; Lide 2003)
Boiling Point (°C):
254 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
142 (calculated-density, liquid molar volume, Chiou 1985)
179.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.0 (Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)
16.95 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.14 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 156 J/mol K), F: 0.602 (mp at 47.5°C)
0.608 (25°C, Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4.31 (shake flask-UV, Yalkowsky et al.)
3.42 (shake flask-GC, Könemann 1981)
4.32 (recommended, Horvath 1982)
3.50 (22°C, Verschueren 1983)
12.2 (generator column-GC/ECD, Miller et al. 1984, 1985)
7.18 (23°C, shake flask-GC, Chiou 1985)
5.92 (shake flask-HPLC, Banerjee et al. 1984)
4.33 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
12.2 (generator column-GC, Doucette & Andren 1988)
3.27 (shake flask-GC/ECD, Kim & Saleh 1990)
12.0 (shake flask-GC, Boyd et al. 1998)
1.40, 2.11, 2.80, 5.25 (5, 15, 25, 35°C, estimated- RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (68.5°C, summary of literature data, temp range 68.5–254.0°C, Stull 1947)
8.76 (extrapolated-Antoine eq., supercooled liquid P_L, Weast 1972–73)
5.21 (calculated-Antoine eq. from Weast 1972–73, converted to solid P_S,; Mackay & Shiu 1981)
log (P/mmHg) = [–0.2185 × 12872.5/(T/K)] + 8.251056; temp range 68.5–254°C (Antoine eq., Weast 1972–73)
4.017, 3.49 (P_{GC} by GC-RT correlation with different GC columns, Bidleman 1984)
8.0 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus}, Bidleman 1984)
6.285 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
2.44 (supercooled liquid P_L, extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.7082 – 1517.2/(–117.384 + T/K); temp range 331–527 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
5.60 (selected, supercooled liquid P_L, Suntio et al. 1988b; quoted, Ballschmiter & Wittlinger 1991)
8.0 (supercooled P_L, converted from literature P_S with ΔS_{fus}, Hinckley et al. 1990)
4.02 (P_{GC} by GC-RT correlation, Hinckley et al. 1990)
12.1 (supercooled liquid P_L, GC-Kovás retention indices correlation; Spieksma et al. 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
70 (gas stripping-GC, Oliver 1985)
62.0* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)
289 (modified EPICS method-GC, Ryu & Park 1999)
58.5 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 5.014 – 1945/(T/K) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.:
4.72 (Leo et al. 1971)
4.46 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)
4.37 (shake flask-GC, Watarai et al. 1982)
4.94 (TLC-RT correlation, Bruggeman et al. 1982)
4.75 (shake flask-GC, Bruggeman et al. 1982)
4.41 (HPLC-k′ correlation, Hammers et al. 1982)
4.55 (generator column-GC, Miller et al. 1984)
4.60 (shake flask-GC, Chiou 1985)
4.65 (HPLC-RV/MS, Burkhard & Kuehl 1986)
4.61* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)
4.60 (shake flask-GC, Pereira et al. 1988)
4.635 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
4.54 (recommended, Sangster 1993)
4.64 (recommended, Hansch et al. 1995)
4.41 ± 0.06* (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)
log K_{OW} = 0.6978 – 21100/[2.303·R(T/K)], temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
4.30* (estimated RP-HPLC-k′ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partoition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
5.64*; 5.74 (generator column-GC; measured range –10 to 20°C, calculated, Harner & Mackay 1995)
log K_{OA} = –5.3 + 3254/(T/K); ΔH_{OA} = 62.3 kJ/mol (Harner & Mackay 1995)
5.64 (calculated-S_{oct} and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF at 25°C or as indicated:
4.86 (guppy, lipid basis, Könemann & van Leeuwen 1980)
3.25 (Briggs 1981)
3.36–3.75 mean 3.72; 4.00–4.15 mean 4.08 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
4.80–5.13 (rainbow trout, lipid basis, Oliver & Niimi 1983)
3.72–4.08 (fish, Oliver 1984)
3.70 (15°C, rainbow trout, Banerjee et al. 1984)
3.41–3.93 mean 3.80; 3.49–4.00 mean 3.91 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)
3.72; .89 (rainbow trout, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)
3.38 (fathead minnow, Carlson & Kosian 1987)
4.9–5.4, 5.1; 4.1 (Niagara River plume, range, mean; calculated-K_{OW}, Oliver 1987b)

4.70, 4.74, 4.75, 4.84 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
3.36 (guppy, Van Hoogan & Opperhuizen 1988)
5.46, 5.70, 4.68, 5.30 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.68; 3.79 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption; purge desorption, Koelmans et al. 1993)
3.40 (guppy, steady-state conditions, rate const. ratio k_1/k_2, 96-h exposure, Sijm et al. 1993)
4.70 (guppy, lipid normalized BCF, Sijm et al. 1993)
3.72–4.08; 3.82 (*Oncorhynchus mykiss; Poecilia reticula*, flow through conditions, Devillers et al. 1996)
3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)
4.28 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
3.96; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
3.49 (soil, sorption isotherm, converted from reported log K_{OM} of 3.25, Briggs 1981)
3.27 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
3.16–4.42 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
5.00; 4.90 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
4.1–6.0, 5.2 (suspended sediment, average, Oliver 1987c)
3.52, 3.91, 3.75, 3.48, 3.52 (five soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
3.48–3.91 (soil, batch-equilibration, Kishi et al. 1990)
4.28 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
4.26 (sediment 3.86% OC, batch sorption equilibrium, Koelmans & Lijkelma 1992)
4.39 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)
3.70, 3.64, 3.84 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
4.14 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:
3.25 (soil, sorption isotherm, shake flask-GC, soil organic matter, Briggs 1981)
4.90 (Niagara River-organic matter, Oliver & Charlton 1984)
4.90–5.40; 5.10; 4.10; 4.50 (Niagara-River plume: range; average; calculated-K_{OW}, algae > 50 μm, Oliver 1987b)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation: dechlorination pseudo-first order rate constant $k = 1.455\ d^{-1}$ with $t_{1/2} = 0.5$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 140\ h^{-1}$; $k_2 = 0.021\ h^{-1}$ (rainbow trout, 15°C, Banerjee et al. 1984)
$k_1 = 670\ mL\ g^{-1}\ d^{-1}$; $k_2 = 0.29\ d^{-1}$ (guppy, van Hoogan & Opperhuizen 1988)
$k_1 = 670 \pm 180\ L\ kg^{-1}\ d^{-1}$; $k_2 = 0.29 \pm 0.06\ d^{-1}$ (guppies, 96-h exposure., Sijm et al. 1993)
$k_1 = 1807.8\ h^{-1}$; $k_2 = 0.304\ h^{-1}$ (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)
$k_1 = 141\ mL\ g^{-1}\ d^{-1}$, $k_2 = 1.5\ d^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:
Air:
Surface Water:
Groundwater:

Sediment: dechlorination $t_{1/2}$ = 1.8 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota: biological half-lives, $t_{1/2}$ = 3 d in sunfish and $t_{1/2}$ = 2 d in guppy for tetrachlorobenzenes (Niimi 1987); $t_{1/2}$ < 5 d in worms at 8°C (Oliver 1987a).

TABLE 6.1.1.8.1

Reported vapor pressures and Henry's law constants of 1,2,3,4-tetrachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C\cdot\log(T/K)$	(4)		

Vapor pressure		**Henry's law constant**	
Stull 1947		**ten Hulscher et al. 1992**	
summary of literature data		**gas stripping-GC**	
t/°C	**P/Pa**	**t/°C**	**H/(Pa m³/mol)**
68.5	133.3	14.8	48.5
99.6	666.6	20.0	62.0
114.7	1333	20.1	52.0
131.2	2666	22.1	68.1
149.2	5333	24.1	70.9
160.0	7999	34.8	129.9
175.7	13332	50.0	276.2
198.0	26664		
225.5	53329	temp dependence eq.	
254.0	101325	$\ln K_{AW} = A - B/(T/K)$	
		A	22.156
mp/°C	46.5	B	5532.84

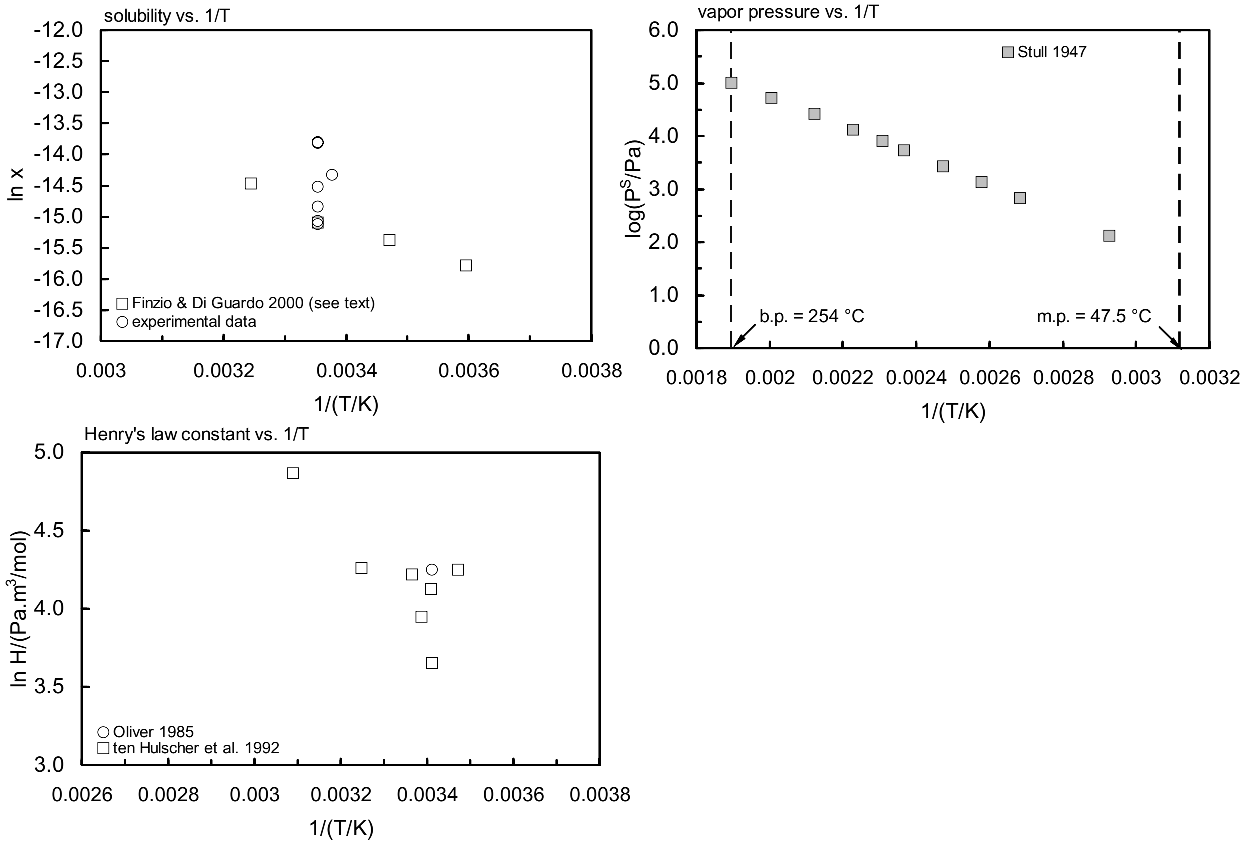


FIGURE 6.1.1.8.1 Logarithm of mole fraction solubility, vapor pressure and Henry's law constant versus reciprocal temperature for 1,2,3,4-tetrachlorobenzene.

TABLE 6.1.1.8.2
Reported octanol-water and octanol-air partition coefficients of 1,2,3,4-tetrachlorobenzene at various temperatures

log K_{OW}						log K_{OA}	
Opperhuizen et al. 1988		Bahadur et al. 1997		Finizio & Di Guardo 2001		Harner & Mackay 1995	
shake flask-GC/ECD		shake flask-GC/ECD		GC-RT correlation		generator column-GC	
t/°C	log K_{OW}	t/°C	log K_{OW}	t/°C	log K_{OW}	t/°C	log K_{OA}
13	4.83	5	4.65	5	4.52	25	5.64
19	4.61	15	4.53	15	4.4	–10	7.076
28	4.37	25	4.41	25	430	0	6.64
33	4.66	35	4.28	35	4.11	9.88	6.213
		45	4.15			19.85	5.818
$\Delta H/(kJ\ mol^{-1}) = -26.3$		enthalpy of transfer				$\Delta H_{OA}/(kJ\ mol^{-1}) = 62.03$	
		$\Delta H/(kJ\ mol^{-1}) = -21.1$					
		$\log K_{OW} = A - \Delta H/2.303RT$				$\log K_{OA} = A + B/T$	
		A	0.6978			A	–5.3
		ΔH	–21100			B	3254

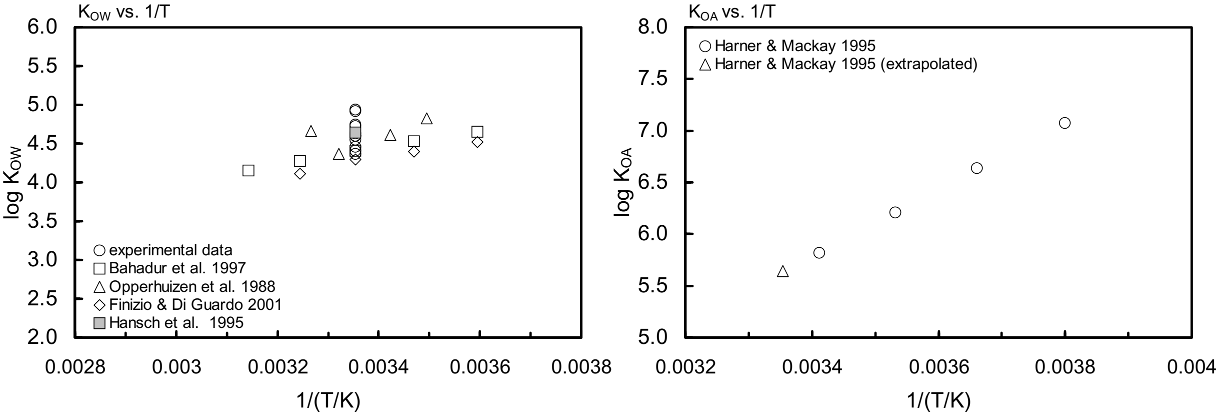
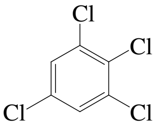


FIGURE 6.1.1.8.2 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for 1,2,3,4-tetrachlorobenzene.

6.1.1.9 1,2,3,5-Tetrachlorobenzene



Common Name: 1,2,3,5-Tetrachlorobenzene
Synonym:
Chemical Name: 1,2,3,5-tetrachlorobenzene
CAS Registry No: 634-90-2
Molecular Formula: $C_6H_2Cl_4$
Molecular Weight: 215.892
Melting Point (°C):
54.5 (Weast 1972–73; 1982–83; Lide 2003)
Boiling Point (°C):
246 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
179.6 (calculated-Le Bas method at normal boiling point)
141.0 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.0 (Miller et al. 1984; Chickos et al. 1999)
19.32 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
58.576 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.514 (mp at 54.5°C)
0.556 (Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3.50 (shake flask-UV, Yalkowsky et al. 1979)
4.02 (shake flask-LSC, Banerjee et al. 1980)
4.11, 17.1 (LSC-^{14}C, calculated-K_{OW}, Veith et al. 1980)
2.48 (shake flask-GC, Könemann 1981)
3.51 (recommended, Horvath 1982)
2.40 (22°C, Verschueren 1983)
5.10 (shake flask-HPLC, Banerjee 1984)
2.89 (generator column-GC/ECD, Miller et al. 1984, 1985)
3.23 (shake flask-GC, Chiou 1985)
3.46 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
4.32 (generator column-GC, Doucette & Andren 1988)
4.32 (shake flask-GC/ECD, Kim & Saleh 1990)
4.52 (shake flask-GC/ECD, Tam et al. 1996)
3.44 ± 0.15*, 3.79 ± 0.23 (generator column-GC/ECD, shake flask-GC at 27°C, Shiu et al. 1997)
$\ln x = -4.4222 - 3162.74/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (58.2°C, summary of literature data, temp range 58.2–246°C, Stull 1947)
18.6 (extrapolated-supercooled liquid P_L, Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 11982.1/(T/K)] + 7.925176$; temp range 58.2–246°C (Antoine eq., Weast 1972–73)
9.80 (solid P_S, calculated from extrapolated vapor pressure P_L with a fugacity ratio correction, Mackay & Shiu 1981)

5.085 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
17.2; 9.56 (extrapolated-Antoine eq., supercooled liquid P_L, converted to P_S, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.7756 – 2394/(–17.85 + T/K); temp range 331–519 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
15.1 (supercooled liquid P_L, GC-Kovás retention indices correlation; Spieksma et al. 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
159 (batch stripping-GC, Mackay & Shiu 1981)
99 (20°C, gas stripping-GC, ten Hulscher et al. 1992)
160 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.:
4.50, 4.92 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
4.46 (HPLC-RT correlation, Veith et al. 1979b)
4.46, 5.0 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
4.52 (shake flask-LSC, Banerjee et al. 1980)
5.05 (head-space GC, Hutchinson et al. 1980)
4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)
4.56 (shake flask-GC, Watarai et al. 1982)
4.53 (HPLC-k′ correlation, Hammers et al. 1982)
4.51 (generator-column-GC/ECD, Miller et al. 1984; 1985)
4.61–4.73 (HPLC-RV correlation, Garst 1984)
4.59 (shake flask-GC, Chiou 1985)
4.59 (shake flask-GC, Pereira et al. 1988)
4.658 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
4.63 (recommended, Sangster 1993)
4.66 (recommended, Hansch et al. 1995)
4.55* ± –0.02 (shake flask-GC/ECD, Bahadur et al. 1997)
log K_{OW} = 1.0159 – 20200/[2.303·R(T/K)]; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
5.55 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)
5.78* (20°C, HPLC-k′ correlation, measured range 10–50°C, Su et al. 2002)
log K_{OA} = 66320/(2.303·RT) – 6.086; temp range 10–50°C (HPLC-k′ correlation, Su et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:
3.26 (fathead minnow, Veith et al. 1979b)
4.86 (guppy-lipid basis, Könemann et al. 1979)
4.15, 4.86 (guppy-lipid basis, Könemann & van Leeuwen 1980)
3.26 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
4.80–5.13 (rainbow trout, lipid base, Oliver & Niimi 1983)
3.46 (22°C, bluegill sunfish, Banerjee et al. 1984)
3.59 (fish, calculated-concentration ratio C_A/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
4.73 (guppy-lipid phase, 12 to 31-d exposure studies, Gobas et al. 1989)
5.05, 5.20, 4.27, 4.90 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.64–4.89 (*Poecilia reticula*, quoted lit., flow through conditions, Devillers et al. 1996)
3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)
4.27 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
4.11; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
3.49 (soil, sorption isotherm, converted from reported log K_{OM} of 3.25, Briggs 1981)

3.20	(Koch 1983)
4.25	(Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
3.94 ± 0.33	(suspended particulates in coastal waters, Masunaga et al. 1996)

Sorption Partition Coefficient, log K_{OM}:

3.20, 2.98	(quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: dechlorination pseudo-first order rate constant $k = 0.639\ d^{-1}$ with $t_{½} = 1.1$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 15000\ d^{-1}$; $k_2 = 0.26\ d^{-1}$ (guppy, Könemann & van Leeuwen 1980)
$k_1 = 74\ h^{-1}$; $k_2 = 0.026\ h^{-1}$ (bluegill sunfish, Banerjee et al. 1984)
$k_1 = 33.8\ h^{-1}$; $1/k_2 = 92.0$ h (guppy, Hawker & Connell 1985)
$k_1 = 810\ d^{-1}$ (fish quoted, Opperhuizen 1986)
$\log k_1 = 2.91\ d^{-1}$; $\log 1/k_2 = -0.42$ d (guppy, quoted, Connell & Hawker 1988)
$\log k_1 = 3.00\ d^{-1}$; $\log k_2 = -0.59\ d^{-1}$ (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)
$\log k_2 = -0.58\ d^{-1}$ (fish, calculated-K_{OW}, Thomann 1989)
$k_1 = 1807.8\ h^{-1}$; $k_2 = 0.304\ h^{-1}$ (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)
$k_1 = 131\ mL\ g^{-1}\ d^{-1}$, $k_2 = 1.4\ d^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air:

Surface Water:

Groundwater:

Sediment: dechlorination $t_{½} = 1.8$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota: $t_{½} = 2–4$ d in fish (Veith et al. 1980);
$2 < t_{½} < 4$ d in bluegill sunfish (Barrows et al. 1980).

TABLE 6.1.1.9.1
Reported aqueous solubilities, vapor pressures, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,3,5-tetrachlorobenzene at various temperatures

Aqueous solubility		Vapor pressure		log K_{OW}		log K_{OA}	
Shiu et al. 1997		Stull 1947		Bahadur et al. 1997		Su et al. 2002	
shake flask-GC		summary of literature data		shake flask-GC/ECD		GC-RT correlation	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OW}	t/°C	log K_{OA}
5	1.7	58.2	133.3	5	4.8	10	6.15.
15	2.43	89	666.6	15	4.67	20	5.78
25	3.44	104.1	1333	25	4.55	30	5.43
35	5.08	121.6	2666	35	4.42	40	5.11
45	7.03	140	5333	45	4.33	50	4.8
		142	7999				
ΔH_{sol} = 26.3 kJ/mol		168	13332	enthalpy of transfer		$\Delta H_{OA}/(kJ\ mol^{-1})$ = 66.32	
		193.7	26664	$\Delta H/(kJ\ mol^{-1}) = -20.2$			
		220	53329			log K_{OA} = A + B/2.303RT	
		246	101325	log K_{OW} = A – B/2.303RT		A	–6.086
				A	1.0195	B	66320
		mp/°C	54.5	ΔH	–20200		

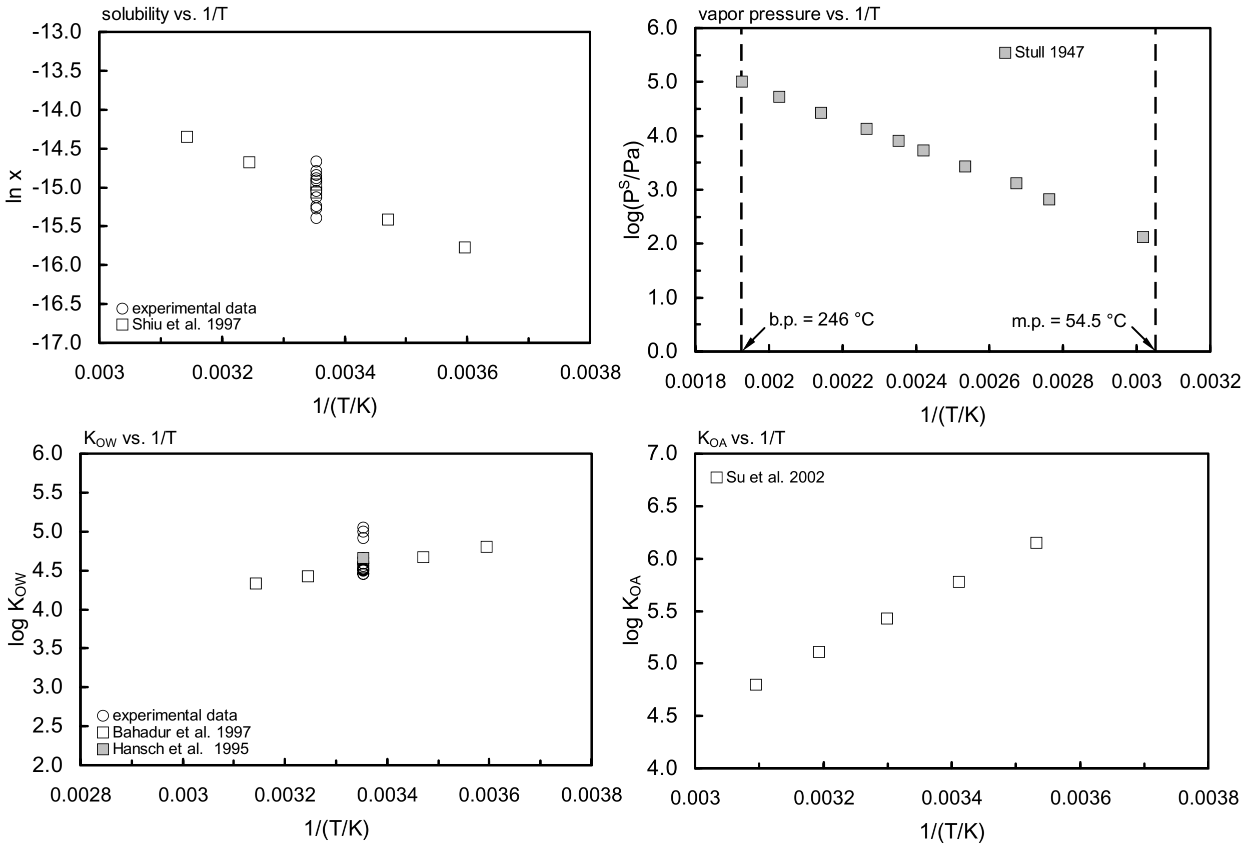
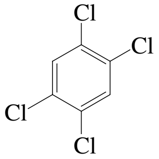


FIGURE 6.1.1.9.1 Logarithm of mole fraction solubility, vapor pressure, K_{OW} and K_{OA} versus reciprocal temperature for 1,2,3,5-tetrachlorobenzene.

6.1.1.10 1,2,4,5-Tetrachlorobenzene



Common Name: 1,2,4,5-Tetrachlorobenzene
Synonym:
Chemical Name: 1,2,4,5-tetrachlorobenzene
CAS Registry No: 95-94-3
Molecular Formula: $C_6H_2Cl_4$
Molecular Weight: 215.892
Melting Point (°C):
139.5 (Lide 2003)
Boiling Point (°C):
244.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.858 (22°C, Weast 1972–1973; Horvath 1982; Lide 2003)
Molar Volume (cm^3/mol):
116.2 (22°C, calculated-density)
179.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.64 (Miller et al. 1984)
24.10 (Ruelle & Kesselring 1993; Chickos et al. 1999)
29.94 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
58.576 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K.), F: 0.0753 (mp at 139.5°C)
0.073 (Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.595 (shake flask-UV, Yalkowsky et al. 1979)
0.29 (shake flask-GC, Könemann 1981)
0.596 (recommended, Horvath 1982)
0.30 (22°C, quoted, Verschueren 1983)
2.35 (generator column-GC/ECD, Miller et al. 1984, 1985)
0.465 (shake flask-HPLC, Banerjee 1984)
0.606 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
0.56 (shake flask-GC/ECD, Kim & Saleh 1990)
0.528* ± 0.018, 0.543 ± 0.016 (generator column-GC/ECD, shake flask-GC at 27°C, Shiu et al. 1997)
2.20 (shake flask-GC, Boyd et al. 1998)
$\ln x = -4.529 - 3708.6/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
5333* (146.0°C, summary of literature data, temp range 146.0–245°C, Stull 1947)
10.1 (extrapolated-Antoine eq., supercooled liquid P_L, Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 12828.8/(T/K)] + 8.282213$; temp range 146–245°C (Antoine eq., Weast 1972–73)
0.72 (P_S converted from P_L of Weast 1972–73, Mackay & Shiu 1981)
0.20 (evaporation rate, Dobbs & Cull 1982)
2.163 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)

2.98, 0.22 (supercooled liquid P_L, solid P_S, Stephenson & Malanowski 1987)
log (P_L/kPa) = 9.1357 – 4642.36/(132.952 + T/K); temp range 419–518 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
7.497 (GC-RT correlation, Watanabe & Tatsukawa 1989)
0.615 (calculated-UNIFAC activity coefficients, Banerjee et al. 1990)
15.1; 12.5 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
0.392* (24.65°C, torsion, mass-loss effusion, measured range 17–32.5°C, Blok et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
101 (gas stripping-GC, Oliver 1985)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
4.72 (Leo et al. 1971)
4.82, 4.56 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)
4.46 (shake flask-GC, Watarai et al. 1982)
4.52 (HPLC-k′ correlation, Hammers et al. 1982)
4.51 (generator column-GC/ECD, Miller et al. 1984, 1985)
4.70 (shake flask-GC, Chiou 1985)
4.60 (HPLC-k′ correlation, Mailhot 1987)
5.16 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
4.604 (slow stirring-GC, De Bruijn et al. 1989)
5.16 (calculated-fragment const., De Bruijn et al. 1989)
4.70 (shake flask-GC, Pereira et al. 1988)
4.63 (recommended, Sangster 1993)
4.70 (recommended, Hansch et al. 1995)
4.97–5.10 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1998)
4.44* (estimated- RP-HPLC-k′ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.:
5.63*; 5.81 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
log K_{OA} = –5.0 + 3176/(T/K); ΔH_{OA} = 60.8 kJ/mol (Harner & Mackay 1995)
5.62, 5.63 (calculated-S_{oct} and vapor pressure P, quoted lit., Abraham et al. 2001)

Bioconcentration Factor, log BCF at 25°C or as indicated:
0.20 (rats, adipose tissue, Geyer et al. 1980)
3.65 (fish, flowing water, Kenaga & Goring 1980; Kenaga)
3.36–3.79 mean 3.72; 4.04–4.18 mean 4.11 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
4.80–5.13 (rainbow trout, lipid base, Oliver & Niimi 1983)
3.72–4.11 (fish, Oliver 1984)
2.80 (Tadokoro & Tomita 1987)
3.89 (green algae, Mailhot 1987)
4.08 (guppy, concn ratio of C_{fish}/C_{water}, Opperhuizen & Voors 1987)
5.05, 5.20, 4.27, 4.90 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
2.76 (*picea omorika*, Reischl et al. 1989)
3.61, 4.70 (American flagfish: whole fish, fish lipid, Smith et al. 1990)
3.20 (fish, calculated, Figueroa & Simmons 1991)
3.72–4.11; 3.61 (*Oncorhynchus mykiss; Jordanella floridae*, quoted lit., flow through conditions, Devillers et al. 1996)
3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)
3.72, 4.80; 3.517, 3.417 (quoted: whole fish, lipid content; calculated-MCI χ, calculated-K_{OW}, Lu et al. 1999)

3.89; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

3.20 (Kenaga 1980a)
3.49 (soil, sorption isotherm, converted from reported log K_{OM} of 3.25, Briggs 1981)
3.36 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
3.24–4.50 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
5.10; 4.70 (field data of sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
2.79 (McLaurin sandy loam, OC 0.66%, pH 4.43, batch equilibrium-sorption isotherm, Walton et al. 1992)
3.94 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)
3.48 (soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: $t_{½}$ = 763.1–7631 h, based on photooxidation half-life in air (Howard et al. 1991)
Hydrolysis: base rate constant k < 0.9 M^{-1} h^{-1} at 25°C with a calculated $t_{½}$ > 900 yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)
 first order hydrolysis $t_{½}$ > 879 yr (Howard et al. 1991)
Biodegradation: $t_{½}$(aerobic) = 672–4320 h, based on unacclimated aerobic screening test data; $t_{½}$(anaerobic) = 2880–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
 dechlorination pseudo-first order k = 0.037 d^{-1} with $t_{½}$ = 18.7 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
 k_1 = 1490 mL g^{-1} d^{-1}; k_2 = 0.14 d^{-1} (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)
 k_1 = 1630 d^{-1}, 171000 d^{-1}; k_2 = 0.4 d^{-1}, 0.34 d^{-1} (American flagfish: whole fish, fish lipid, Smith et al. 1990)
 k_2 = 0.4 d^{-1}, 2.35 d^{-1} (American flagfish: bioconcentration data, toxicity data, Smith et al. 1990)
 k_1 = 1807.8 h^{-1}; k_2 = 0.304 h^{-1} (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{½}$ = 763.1–7631 h, based on photooxidation half-life in air (Howard et al. 1991)
Surface Water: hydrolysis $t_{½}$ > 900 yr at pH 7 and 25°C (Ellington et al. 1988)
 $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Groundwater: $t_{½}$ = 1344–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Sediment: dechlorination $t_{½}$ = 18.7 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Soil: $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Biota: $t_{½}$ < 5 d in worms at 8°C (Oliver 1987a);
 biological $t_{½}$ = 3 d in sunfish, $t_{½}$ = 2 d in guppy for tetrachlorobenzenes (Niimi 1987);
 $t_{½}$ = 33 d in *Picea omorika* (Reischl et al. 1989);
 $t_{½}$ = 1.72 d clearance from American flagfish (Smith et al. 1990);
 elimination $t_{½}$ = 2.01 d from earthworm in water (Belfroid et al. 1993);
 elimination $t_{½}$ = 0.204 d and 2.63 d in a two-phase kinetics for earthworm in OECD soil (Belfroid et al. 1994).

TABLE 6.1.1.10.1
Reported aqueous solubilities and vapor pressures of 1,2,4,5-tetrachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C\cdot\log(T/K)$	(4)		

Aqueous solubility		Vapor pressure					
Shiu et al. 1997		Stull 1947		Blok et al. 2001			
shake flask-GC		summary of literature data		torsion, mass loss effusion		static-diaphragm manometer	
t/°C	$S/g\cdot m^{-3}$	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
5	0.298	146.0	5333	16.85	0.155	99.74	328
15	0.322	157.7	7999	19.45	0.212	104.82	461
25	0.528	173	13332	22.05	0.289	108.83	612
35	0.739	196	26664	24.65	0.392	113.82	844
45	1.127	220.5	53329	27.25	0.528	117.74	1100
		245	101325	29.85	0.707	121.82	1140
ΔH_{sol} = 30.8 kJ/mol				32.45	0.943	125.84	1820
		mp/°C				129.82	2310
				$\Delta H_{subl}/(kJ\ mol^{-1})$ = 82.10		132.79	2770
				at 353 K		136.82	3500

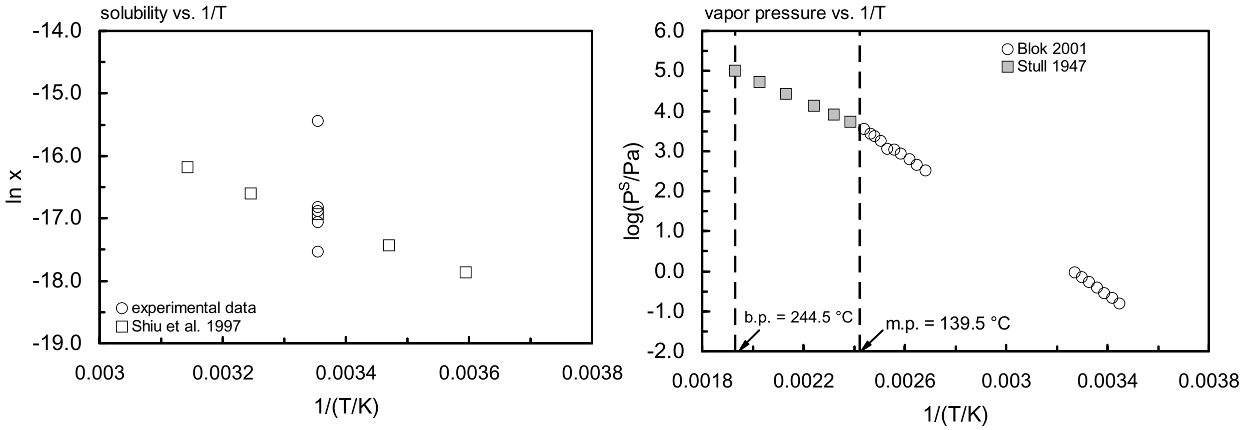


FIGURE 6.1.1.10.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,4,5-tetrachlorobenzene.

TABLE 6.1.1.10.2
Reported octanol-water partition coefficients and octanol-air partition coefficients of 1,2,4,5-tetrachlorobenzene at various temperatures

log K_{OW}		log K_{OA}	
Finizio & Di Guardo 2001		Harner & Mackay 1995	
GC-RT correlation		generator column-GC	
t/°C	log K_{OW}	t/°C	log K_{OA}
5	4.63	25	5.63
15	4.54	–10	7.056
25	4.44	0	6.622
35	4.26	9.88	6.204
		19.85	5.829
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 60.8$	
		$\log K_{OA} = A + B/T$	
		A	–5.0
		B	3176

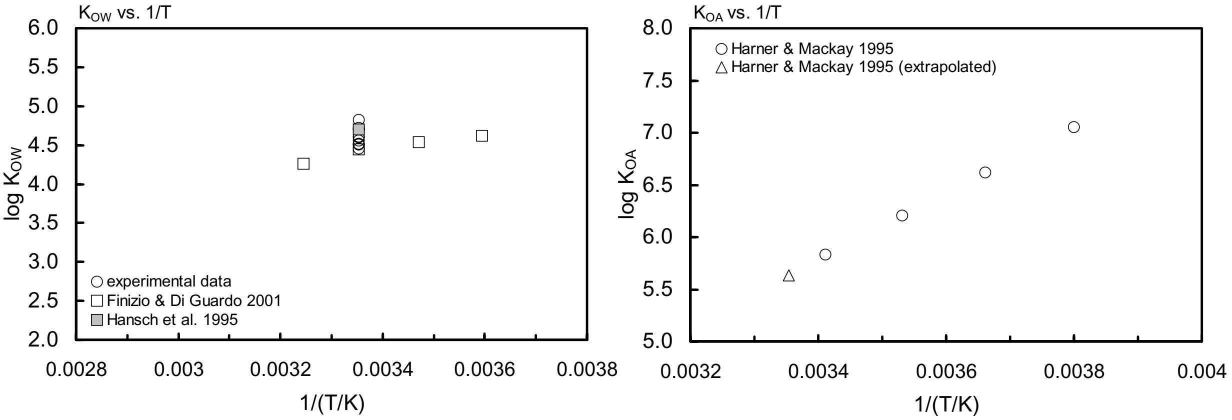
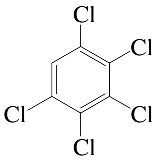


FIGURE 6.1.1.10.2 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for 1,2,4,5-tetrachlorobenzene.

6.1.1.11 Pentachlorobenzene



Common Name: Pentachlorobenzene
Synonym:
Chemical Name: Pentachlorobenzene
CAS Registry No: 608-93-5
Molecular Formula: C_6HCl_5
Molecular Weight: 250.337
Melting Point (°C):
86 (Weast 1972–73; Lide 2003)
Boiling Point (°C):
277 (Weast 1972–72; Lide 2003)
Density (g/cm^3 at 20°C):
1.8342 (16.5°C, Weast 1972–73; Horvath 1982)
Molar Volume (cm^3/mol):
136.5 (16.5°C, calculated-density, Weast 1972–73; Horvath 1982)
166 (liquid molar volume, Chiou 1985)
200.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.585 (Miller et al. 1984)
20.60 (Ruelle et al. 1993; Chickos et al. 1999)
20.1 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
57.74 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K.), F: 0.252 (mp at 86°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.56 (shake flask-UV, Yalkowsky et al. 1979)
1.33 (shake flask-LSC, Banerjee et al. 1980)
0.135 (Kenaga & Goring 1980; Kenaga 1980a)
1.34 (shake flask-LSC-^{14}C, Veith et al. 1980)
0.24 (shake flask-GC, Könemann 1981)
0.562 (recommended, Horvath 1982)
0.831 (generator column-GC/ECD, Miller et al. 1984, 1985)
0.385 (23°C, shake flask-GC, Chiou 1985)
0.180 (generator column-GC/ECD, Opperhuizen et al. 1985)
0.552 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
3.46 (calculated-K_{OW} and HPLC-RT correlation, Chin et al. 1986)
0.419* ± 0.018, 0.447 ± 0.014 (generator column-GC/ECD, shake flask-GC/ECD at 27°C, Shiu et al. 1997)
0.87 (shake flask-GC, Boyd et al. 1998)
$\ln x = -3.61482 - 4093.10/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
2.75, 3.50 (supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133* (98.6°C, summary of literature data, temp range 98.6–276°C, Stull 1947)

0.889 (extrapolated-Antoine eq., supercooled liquid P_L, Weast 1972–73)
0.219 (P_S calculated from P_L of Weast 1972–73; Mackay & Shiu 1981)
log (P/mmHg) = [–0.2185 × 15124.2/(T/K)] + 8.907497; temp range 98.6–276°C (Antoine eq., Weast 1972–73)
1.44 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
1.08, 0.28 (supercooled liquid P_L, solid P_S, Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 8.00795 – 3325.33/(4.814 + T/K); temp range 371–549 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
1.718 (GC-RT correlation, Watanabe & Tatsukawa 1989)
2.49; 2.19 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
0.212; 0.39* (25°C extrapolated; 30.3°C, static method-pressure gauge, measured range 30.3–179°C, Polednicek et al. 1996)
ln (P_S/Pa) = 30.4445 – 8654.67/[(T/K) – 27.6534]; temp range 303.45–353.17 K (solid, Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
ln (P_L/Pa) = 23.4783 – 6188.33/[(T/K) – 34.6922]; temp range 371.8–452.29 K (liquid, Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
0.11* (20°C, recommended, summary of literature data, temp range 233.15–503.15 K, Roháč et al. 1999)
ln [(P_S/Pa)/67.0] = [1 – (T/K)/357.0)·exp{3.431590 – 1.8864070 × 10^{-4}·(T/K)}; temp range 300–353 K (Cox eq., solid, recommended, Roháč et al. 1999)
ln [(P_L/Pa)/67.0] = [1 – (T/K)/357.0)·exp{3.419638 – 1.1673259 × 10^{-3}·(T/K) + 7.7842905 × 10^{-7}(T/K)^2}; temp range 365–452 K (Cox eq., liquid recommended, Roháč et al. 1999)
log (P/kPa) = 15.6174 – 4831.4/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
1.2, 1.0 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
log (P_L/Pa) = –3220/(T/K) + 10.87 (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant (Pa m^3/mol at 25°C or reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
71.9 (gas stripping-GC, Oliver 1985)
59.0* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)
52.6 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 5.607 – 2132/(T/K) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
74, 70 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
log K_{AW} = –2026/(T/K) + 5.27 (LDV linear regression of literature data, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
5.79 (calculated-fragment const., Yalkowsky et al. 1979)
4.88, 5.52 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
4.94 (shake flask-LSC, Banerjee et al. 1980)
4.94, 5.29 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
5.17 (shake flask-GC, Watarai et al. 1982)
5.06 (HPLC-k′ correlation, Hammers et al. 1982)
5.69 (HPLC-RT correlation, Bruggeman et al. 1982)
5.03 (generator column-GC/ECD, Miller et al. 1984; 1985)
5.17 (shake flask-HPLC, Banerjee 1984)
5.11–5.21 (HPLC-RV correlation, Garst 1984)
5.20 (shake flask-GC, Chiou 1985)
4.97 (calculated-K_{OW} and HPLC-RT correlation, Chin et al. 1986)
6.12 (HPLC-k′ correlation, De Kock & Lord 1987)
5.47 (HPLC-RT correlation, Doucette & Andren 1988)
5.20 (shake flask-GC, Pereira et al. 1988)
5.05* (19°C, shake flask-GC, measured range 13–33°C, Opperhuizen et al. 1988)
5.183 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
5.17 (recommended, Sangster 1993)
5.18 (recommended, Hansch et al. 1995)
4.94* ± 0.03 (shake flask-GC/ECD, Bahadur et al. 1997)

log K_{OW} = 0.9255 – 22800/[2.303·R(T/K)]; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
5.67–5.78 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1998)
5.08, 5.19 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
6.27*; 6.46 (generator column-GC, measured range –10 to 20°C, calculated, Harner & Mackay 1995)
7.93, 7.418, 6.931, 6.539 (–10, 0, 10, 18.7°C, generator column-GC, Harner & Mackay 1995)
log K_{OA} = –6.2 + 3722.3/(T/K); temp range –10 to 20°C, ΔH_{OA} = 72.3 kJ/mol (generator column-GC, Harner & Mackay 1995)
6.50 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
6.49, 6.27 (calculated-S_{oct} and vapor pressure P, quoted lit., Abraham et al. 2001)
6.90, 6.73 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF at 25°C or as indicated:
3.89 (trout muscle, Neely et al. 1974)
3.70 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980a)
5.40 (guppy, lipid content, Könemann et al. 1979)
3.53 (bluegill sunfish, Veith et al. 1980)
3.53 (bluegill sunfish, whole body, flow system, Barrows 1980)
5.41 (guppy, lipid basis, Könemann & van Leeuwen 1980)
3.84 (fish, flowing water, Garten & Trabalka 1983)
3.46–4.15 mean 4.11; 4.26–4.36 mean 4.30 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
5.19–5.36 (rainbow trout, lipid basis, Oliver & Niimi 1983)
4.11–4.30 (rainbow trout, Oliver 1984)
3.71 (22°C, bluegill sunfish, 1.5% lipid, Banerjee et al. 1984)
3.65; 3.86 (15°C, rainbow trout, 1.8% lipid; guppy, 2.8% lipid, Banerjee et al. 1984)
3.60; 3.49 (algae: exptl.; calculated, Geyer et al. 1984)
3.65 (algae, Freitag et al. 1984; Halfon & Reggiani 1986)
3.48 (fish, Freitag et al. 1984; Halfon & Reggiani 1986)
3.48, 3.65, 4.16 (fish, algae, activated sludge, Freitag et al. 1985)
4.23 (guppy, calculated-rate constants ratio k_1/k_2, Opperhuizen et al. 1985)
3.92 (fathead minnow, Carlson & Kosian 1987)
2.83, 2.65 (human fat, Geyer et al. 1987)
4.28, 4.30 (worm, fish, Oliver 1987a)
3.36–3.42 (fish, Tadokoro & Tomita 1987)
5.46 (guppy, lipid weight base, 12 to 31-d exposure studies, Gobas et al. 1989)
3.87 (*picea omorika*, Reischl et al. 1989)
5.33 (fish, calculated-K_{OW}, Thomann 1989)
4.14, 2.96, 4.23 (fish, Connell & Hawker 1988; Hawker 1990)
5.11, 5.18, 5.20, 5.28 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
3.67 (guppy, Van Hoogan & Opperhuizen 1988)
5.93, 6.12, 4.96, 5.57 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
4.22 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption, Koelmans et al. 1993)
3.70 (guppy, steady-state conditions, rate const. ratio k_1/k_2, 96-h exposure, Sijm et al. 1993)
5.00 (guppy, lipid normalized BCF, Sijm et al. 1993)
4.11–4.30; 2.94–4.36; 3.53 (*Oncorhynchus mykiss; Poecilia reticulata; Lepomis macrochirus*, quoted lit., flow through conditions, Devillers et al. 1996)
5.22–5.50 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
4.11, 5.19; 3.797, 3.877 (quoted: whole fish, lipid content; calculated-MCI χ, calculated-K_{OW}, Lu et al. 1999)
4.09; 3.96 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

4.11 (Kenaga 1980a)
5.30; 5.40 (field data of Lake Ontario sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
4.60 (bottom sediment, Karickhoff & Morris 1985)
4.9–6.2, 5.8 (suspended sediment, average, Oliver 1987c)
5.7 (algae > 50 μm, Oliver 1987c)
5.50–5.90, 5.70 (Niagara River plume: range, average, Oliver 1987b)
4.49 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
4.68 (lake sediment 2.5% OC, batch sorption equilibrium, Schrap et al. 1994)
4.59 ± 0.41 (suspended particulates in coastal waters, Masunaga et al. 1996)
4.91 (sediment: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: $t_{½}$ = 1088–10877 h, based on estimated rate constant for the vapor phase reaction with OH radicals in air (Howard et al. 1991)
Hydrolysis: base rate constant $k < 0.9\ M^{-1}\ h^{-1}$ at 25°C with a calculated $t_{½}$ > 900 yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)
 first order $t_{½}$ > 879 yr (Howard et al. 1991)
Biodegradation: $t_{½}$(aerobic) = 4656–8280 h, based on estimated unacclimated aerobic soil grab sample data; $t_{½}$(anaerobic) = 18642–33120 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
 dechlorination pseudo-first order rate constant $k = 0.557\ d^{-1}$ with $t_{½}$ = 1.2 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 18.76\ h^{-1}$; $k_2 = 0.00238\ h^{-1}$ (trout, Neely et al. 1974)
$k_1 = 22000\ d^{-1}$; $k_2 = 0.14\ d^{-1}$ (guppy, Könemann & van Leeuwen 1980)
$k_1 = 130\ d^{-1}$; $k_2 = 0.15\ d^{-1}$ (guppy, Bruggeman et al. 1984)
$k_1 = 110\ h^{-1}$; $k_2 = 0.021\ h^{-1}$ (22°C, bluegill sunfish, Banerjee et al. 1984)
$k_1 = 170\ h^{-1}$; $k_2 = 0.036\ h^{-1}$ (15°C, rainbow trout, Banerjee et al. 1984)
$k_1 = 98\ h^{-1}$; $k_2 = 0.014\ h^{-1}$ (15°C, guppy, Banerjee et al. 1984)
$k_1 = 5.4\ h^{-1}$; $1/k_2 = 160$ h (guppy, quoted, Hawker & Connell 1985)
$k_1 = 1400\ d^{-1}$; $k_2 = 0.078\ d^{-1}$ (guppy, Opperhuizen et al. 1985)
$k_1 = 1200\ d^{-1}$ (fish, quoted, Opperhuizen 1986)
$k_2 = 0.00309, 0.00402\ d^{-1}$ (rainbow trout, calc-fish mean body weight, Barber et al. 1988)
$\log k_1 = 3.08\ d^{-1}$; $\log 1/k_2 = 0.96$ d (fish, quoted, Connell & Hawker 1988)
$k_1 = 710\ mL\ g^{-1}\ d^{-1}$; $k_2 = 0.15\ d^{-1}$ (guppy, Van Hoogan & Opperhuizen 1988)
$\log k_1 = 3.24\ d^{-1}$; $\log k_2 = -0.96\ d^{-1}$ (guppy, 12 to 31-d exposure studies, Gobas et al. 1989a)
$k_1 = 0.049\ h^{-1}$; $k_2 = 0.027\ h^{-1}$ (mayfly-sediment model II, Gobas et al. 1989b)
$\log k_2 = -0.82\ d^{-1}$; $-0.96\ d^{-1}$ (fish, calculated-K_{OW}, Thomann 1989)
$1/k_2 = 9.12, 12.9$ d (guppy, Clark et al. 1990)
$k_1 = 710 \pm 290\ L\ kg^{-1}\ d^{-1}$; $k_2 = 0.15 \pm 0.04\ d^{-1}$ (guppies, 96-h exposure., Sijm et al. 1993)
$k_2 = 0.00116\ d^{-1}$ (18°C earthworm in field-contaminated soil, Belfroid et al. 1995)
$k_1 = (240–290)\ mL\ g^{-1}\ d^{-1}$, $k_2 = (0.3–0.19)\ d^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air: $t_{½}$ = 1088–10877 h, based on estimated rate constant for the vapor phase reaction with OH radicals (Howard et al. 1991)
Surface Water: $t_{½}$ = 4656–8280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Groundwater: $t_{½}$ = 9312–16560 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment: dechlorination $t_{1/2}$ = 1.20 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Soil: $t_{1/2}$ = 4656–8280 h, based on estimated unacclimated aerobic soil grab sample data (Howard et al. 1991)
Biota: $t_{1/2}$ > 7 d in fish (Veith et al. 1980);
$t_{1/2}$ > 7 d in bluegill sunfish (Barrows et al. 1980);
$t_{1/2}$ = 4.6 d in guppy (Bruggeman et al. 1984);
$t_{1/2}$ = 8.9 d in guppy (Opperhuizen et al. 1985);
$t_{1/2}$ < 5 d in worms at 8°C (Oliver 1987a);
biological half-lives, $t_{1/2}$ > 7 d in sunfish, $t_{1/2}$ = 4, 5 and < 5 d in guppy (Niimi 1987);
$t_{1/2}$ = 27 d in *picea omorika* (Reischl et al. 1989);
elimination $t_{1/2}$ = 5.46 d from earthworm in water (Belfroid et al. 1993);
elimination $t_{1/2}$ = 0.53 d and 5.9 d in a two-phase kinetics from earthworm in OECD soil (Belfroid et al. 1994);
elimination $t_{1/2}$ = 0.60 d from earthworm in Volgermeerpolder soil (Belfroid et al. 1995).

TABLE 6.1.1.11.1
Reported aqueous solubilities of pentachlorobenzene at various temperatures

Shiu et al. 1997	
generator column-GC	
t/°C	$S/g\cdot m^{-3}$
5	0.145
15	0.254
25	0.419
35	0.618
45	0.856
shake flask-GC	
27	0.447
ΔH_{sol} = 32.9 kJ/mol	

TABLE 6.1.1.11.2
Reported vapor pressures of pentachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log (P/Pa) = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log (P/mmHg) = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log (P/Pa) = A - B/(C + T/K)$ (3) $\ln (P/Pa) = A - B/(C + T/K)$ (3a)
$\log (P/mmHg) = A - B/(T/K) - C\cdot\log (T/K)$ (4)
$\ln (P/P_o) = (1 - T/T_o)\cdot\exp[\Sigma A_i T^i]$ (5) - Cox eq.

1.

Stull 1947		Polednicek et al. 1996				Roháč et al. 1999	
summary of lit. data		pressure gauge				recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
			solid		liquid		solid
98.6	133	30.3	0.385	98.65	167.99	233.15	0.00001
129.7	666.6	30.3	0.401	98.69	167.56	243.15	0.000066
144.3	1333	40.26	1.163	108.65	285.2	253.15	0.00037
160	2666	40.27	1.167	108.68	284.76	263.15	0.0019
178.5	5333	50.27	3.227	118.82	470.83	273.15	0.0081

(Continued)

TABLE 6.1.1.11.2 *(Continued)*

Stull 1947		Polednicek et al. 1996				Roháč et al. 1999	
summary of lit. data		pressure gauge				recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
190.1	7999	50.27	3.209	118.84	471.55	283.15	0.032
205.5	13332	60.14	8.473	128.85	756.41	293.15	0.11
227	26664	60.16	8.480	128.85	755.7	303.15	0.37
251.5	53329	70.05	20.35	138.9	1189.2	313.15	1.10
276	101325	70.05	20.39	149.01	1820.6	232.15	3.20
		80.02	47.29	159.06	2731.2	333.15	8.40
mp/°C	85.5	25	0.212	169.11	4009.9	343.25	20.8
			extrapolated	179.14	5750.8	353.15	48.9
			solid		liquid	Cox eq.	
		eq. 3a	P/Pa	eq. 3a	P/Pa	eq. 5	P/Pa
		A	30.4445	A	22.4783	A_0	3.431590
		B	8654.67	B	6188.33	$10^{-4}A_1$	–1.8864070
		C	–27.6534	C	–34.6922	A_2	0
						T_o/K	357.0
						P_o/Pa	67.0
						bp/K	558.42
						for temp range 300–353 K	

2.

Roháč et al. 1999					
recommended					
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
continued	liquid				
363.15	97.5	473.15	11440	Cox eq.	
373.15	173.9	483.15	15500	eq. 5	P/Pa
383.15	298.8	493.15	20700	A_0	3.419638
393.15	486.4	503.15	27250	$10^{-3}A_1$	–1.1673259
403.15	799.8	513.15	35430	$10^{-7}A_2$	7.7842905
413.15	1253	523.15	45510	T_o/K	357.0
423.15	1912	533.15	57820	P_o/Pa	67.0
433.15	2848	543.15	72710	bp/K	558.42
443.15	4151	553.15	90570	for temp range 365–452 K	
453.15	5927	563.15	111800		
463.15	8306				

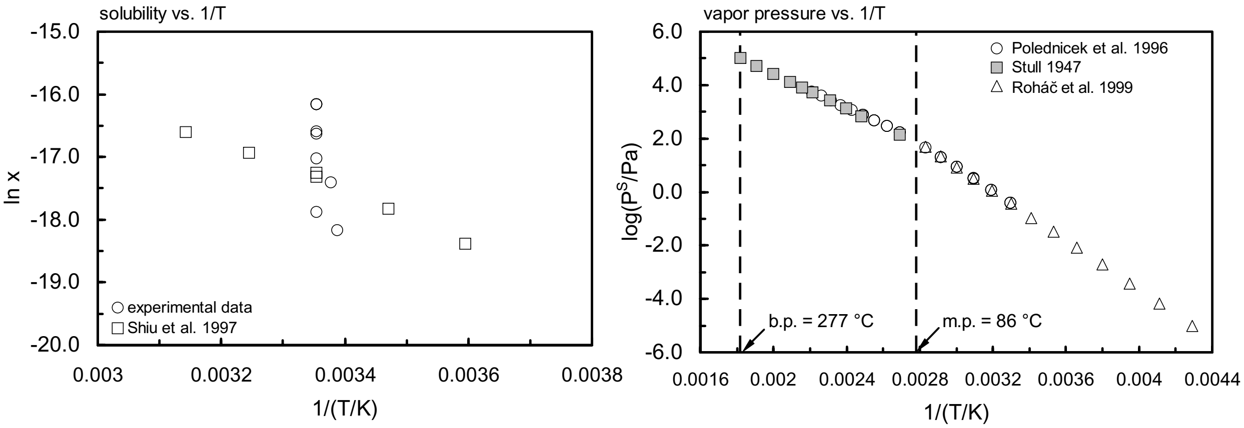


FIGURE 6.1.1.11.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for pentachlorobenzene.

TABLE 6.1.1.11.3
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of pentachlorobenzene at various temperatures

Henry's law constant		log K_{OW}				log K_{OA}	
Ten Hulscher et al. 1992		**Opperhuizen et al. 1988**		**Bahadur et al. 1997**		**Harner & Mackay 1995**	
gas stripping-GC		**shake flask-GC/ECD**		**shake flask-GC/ECD**		**generator column-GC**	
t/°C	**H/(Pa m³/mol)**	**t/°C**	**log K_{OW}**	**t/°C**	**log K_{OW}**	**t/°C**	**log K_{OA}**
14.8	37.4	13	5.2	5	5.2	25	5.64
20	59.0	19	5.05	15	5.06	–10	7.93
20.1	49.4	28	4.70	25	4.94	0	7.418
22.1	68.1	33	4.66	35	4.79	10	6.931
24.1	66.7			45	4.66	18.7	6.539
34.8	124.1						
50.5	276.2	$\Delta H/(kJ\ mol^{-1}) = -30.8$		enthalpy of transfer $\Delta H/(kJ\ mol^{-1}) = -22.8$		$\Delta H_{OA}/(kJ\ mol^{-1}) = 62.03$	
$\ln H = A - B/(T/K)$				$\log K_{OW} = A - \Delta H/2.303RT$		$\log K_{OA} = A + B/T$	
	H/(Pa m³/mol)			A	0.9255.	A	–6.2
A	21.4142			ΔH	–22800	B	3722.3
B	5108						

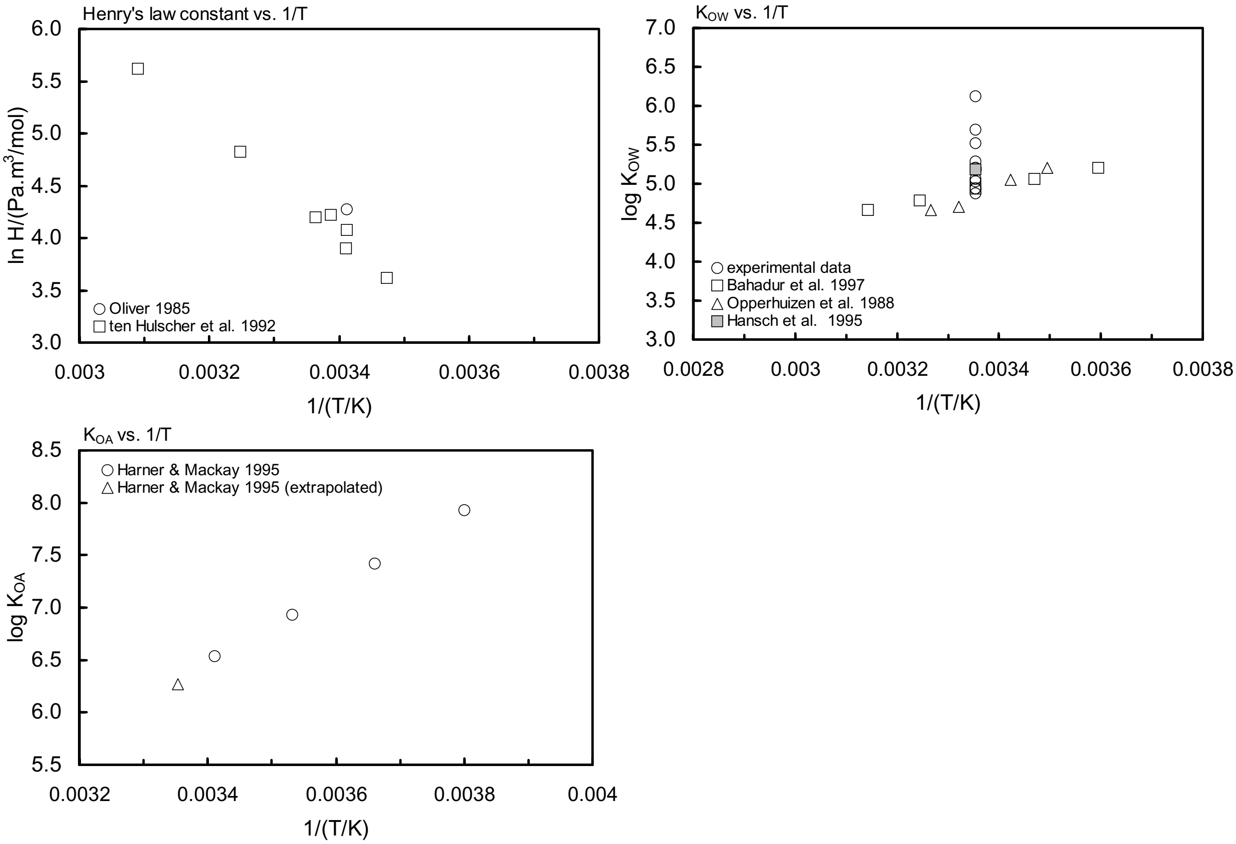
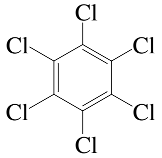


FIGURE 6.1.1.11.2 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for pentachlorobenzene.

6.1.1.12 Hexachlorobenzene



Common Name: Hexachlorobenzene
Synonym: HCB, perchlorobenzene, anticarie, Bunt-cure, Bunt-no-more, Julin's carbon chloride
Chemical Name: hexachlorobenzene
CAS Registry No: 118-74-1
Molecular Formula: C_6Cl_6
Molecular Weight: 284.782
Melting Point (°C):
  228.83 (Lide 2003)
Boiling Point (°C):
  325 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.5691 (23.6°C, Weast 1972–73; Horvath 1982)
  2.004 (23°C, Lide 2003)
Molar Volume (cm^3/mol):
  181.5 (23.6°C, calculated-density, Weast 1972–73; Horvath 1982)
  221.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  23.85 (Plato & Glasgow 1969; Ruelle et al. 1993; Chickos et al. 1999)
  28.74 (Tsonopoulos & Prausnitz 1971)
  22.40 (Miller et al. 1984)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  57.32 (Tsonopoulos & Prausnitz 1971)
  44.77 (Miller et al. 1984)
  47.1 (Hinckley et al. 1990; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.01 (mp at 228.83°C)
  0.009 (Miller et al. 1985; Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.005 (generator column-GC/ECD, Weil et al. 1974)
  0.006 (shake flask-LSC/^{14}C, Lu & Metcalf 1975)
  0.11 (shake flask-nephelometric spectrophotofluorometry, Hollifield 1979)
  0.005 (shake flask-UV, Yalkowsky et al. 1979)
  0.0039 (shake flask-GC, Könemann 1981)
  0.00921, 0.00996 (15, 25°C, generator column/elution method, average values of 6–7 labs., OECD 1981)
  0.0054 (generator column-GC/ECD, Hashimoto et al. 1982)
  0.0012–0.014 (shake flask-GC/ECD, Hashimoto et al. 1982)
  0.005 (recommended, Horvath 1982)
  0.047 (generator column-GC/ECD, Miller et al. 1984; 1985)
  0.005 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
  0.00544* ± 0.00018 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
  0.38 (shake flask-GC, Boyd et al. 1998)
  0.0050 ± 0.00002 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
  $\log [S_L/(mol/L)] = 0.450 - 1212/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
  $\ln x = -8.22956 - 4037.26/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
  0.010* (generator column-GC/ECD, measured range 15–55°C, Oleszek-Kudlak et al. 2004)

0.0273, 0.398 (supercooled liquid: derivation of literature-derived value FAV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (114.1°C, summary of literature data, temp range 114.1–309.4°C, Stull 1947)
0.00028 (extrapolated from Antoine eq., Sears & Hopke 1949)
$\log (P/\text{mmHg}) = 11.397 - 4197.3/(T/K)$; temp range 96–124°C (Rodebush gauge, Sears & Hopke 1949)
$\log (P/\text{mmHg}) = [-0.2185 \times 15199.1/(T/K)] + 8.550497$; temp range 114.4–309.4°C (Antoine eq., Weast 1972–73)
0.0015 (Callahan et al. 1979)
0.0026 (OECD 1979)
0.00145 (20°C, Kiltzer et al. 1979)
0.0023* (gas saturation, measured range 15–45°C, Farmer et al. 1980)
$\log P/\text{mmHg} = 12.94 - 5279/(T/K)$; temp range 15–45°C (gas saturation, Farmer et al. 1980)
0.000453; 0.000167 (Klein et al. 1981)
0.0019* (gas saturation, measured range 10–50°C, OECD 1981)
$\log (P/\text{mmHg}) = 12.237 - 5152.1/(T/K)$; temp range 10–50°C (gas saturation, OECD 1981)
0.00046 (evaporation rate, Dobbs & Cull 1982)
0.00121 (extrapolated-Antoine eq., Gückel et al. 1982)
0.0006 (20°C, evaporation rate and gravimetric method, Gückel et al. 1982)
0.159, 0.122 (P_{GC} by GC-RT correlation with different GC columns, Bidleman 1984)
0.303 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus}, Bidleman 1984)
0.00332 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
0.00205* (41.05°C, gas saturation-GC, measured range 41–100°C, Rordorf 1985)
$\log (P/\text{Pa}) = 12.3243 - 4336.95/[(T/K) - 41.1905]$; temp range 41–100°C (gas saturation, Rordorf 1985)
0.00147, 0.187 (20°C, quoted: solid P_S, supercooled liquid P_L, Bidleman & Foreman 1987)
$\log (P_S/\text{kPa}) = 7.00706 - 2831.85/(-28.25 + T/K)$; temp range 387–502 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 7.35248 - 2786.78/(-61.33 + T/K)$; temp range 502–589 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
0.245 (supercooled liquid P_L, Suntio et al. 1988b)
0.303, 0.127 (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.159, 0.119 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log (P_L/\text{Pa}) = 11.11 - 3582/(T/K)$ (supercooled liquid P_L, GC-RT correlation, Hinckley et al. 1990)
0.00311* (gas saturation, measured range –15 to 40°C, Dickhut et al. 1994)
0.001092* (20°C, gas saturation-GC/ECD, measured range –30 to 40°C, Wania et al. 1994)
$\log (P_S/\text{Pa}) = 10.83 - 4044/(T/K)$; temp range –30 to 40°C (derived from gas saturation data, Wania et al. 1994)
0.367; 0.344 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
$\log (P/\text{mmHg}) = -134.3625 - 1.5459 \times 10^3/(T/K) + 61.748\cdot\log (T/K) - 6.5123 \times 10^{-2}\cdot(T/K) + 2.0872 \times 10^{-5}\cdot(T/K)^2$; temp range 502–825 K (Yaws 1994)
0.0339; 1.46×10^{-3}, 0.141 (liquid P_L from GC-RT correlation; quoted solid P_S, converted to P_L, Donovan 1996)
$(4.6\text{–}26) \times 10^{-4}$, $(1.11\text{–}5.40) \times 10^{-3}$ (quoted exptl. solid P_S ranges: 20°C, Delle Site 1997)
0.271; 0.00821 (P_L supercooled liquid, GC-RT correlation; solid P_S, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 8.42 - 2834/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
0.14, 0.094 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
$\log (P_L/\text{Pa}) = -3530/(T/K) + 10.97$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

131.3 (gas stripping-GC, Atlas et al. 1982)
48.6 (gas stripping-GC, Oliver 1985)
172 (gas stripping-GC, Warner et al. 1987)
41756 (computer value, Yaws et al. 1991)
41.0* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)

ln [H/(Pa m^3/mol)] = 22.7994 – 5630.6/(T/K), temp range 14–50°C (gas stripping-GC, ten Hulscher et al. 1992)
26243, 29587 (26.0, 46.0°C, EPICS-GC, Hansen et al. 1993)
log [H/(Pa m^3/mol)] = 7.97 – 1622/(T/K) (Passivirta et al. 1999)
35.1 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 6.266 – 2377/(T/K) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
52, 65 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

6.18 (Neely et al. 1974)
4.13 (radioisotope tracer-^{14}C, Lu & Metcalf 1975)
6.51 (calculated-fragment constant, Rekker 1977)
4.13 (Hansch & Leo 1979)
5.0, 6.27 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
5.23 (HPLC-RT correlation, Veith et al. 1979b)
6.18 (HPLC-RT correlation, Veith et al. 1979a)
5.44 (shake flask-GC, Briggs 1981)
6.22 (HPLC-RT correlation, McDuffie 1981)
5.56, 5.04–5.92 (shake flask method: mean, range of mean values, OECD 1981)
5.50 (shake flask-GC, Chiou et al. 1982; Chiou 1985)
5.66 (HPLC-RT correlation, Hammers et al. 1982)
5.40 (shake flask-GC, Watarai et al. 1982)
6.13–6.27, 5.66 (range, mean, shake flask method, Eadsforth & Moser 1983)
6.27–6.48, 6.38 (range, mean, HPLC method, Eadsforth & Moser 1983)
5.46, 5.26; 5.47 (Review of HPLC methods; OECD/EEC shake-flask method, Harnisch et al. 1983)
5.47 (generator column-GC/ECD, Miller et al. 1984; 1985)
5.70–5.79 (HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)
6.86 (HPLC/MS correlation, Burkhard et al. 1985)
5.75; 5.60, 5.90 (selected OECD value; HPLC-RV correlation, Brooke et al. 1986)
6.92 (HPLC-k′ correlation, De Kock & Lord 1987)
5.64 (HPLC-k′ correlation, Mailhot 1987)
6.22 (HPLC-RT correlation, Doucette & Andren 1988)
5.7* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)
5.50 (shake flask-GC, Pereira et al. 1988)
5.73 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.44 (recommended, Sangster 1993)
5.73 (recommended, Hansch et al. 1995)
5.46* ± 0.02 (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)
log K_{OW} = 1.1806 – 24.4/[2.303R(T/K)]; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
5.845 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
5.55 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrăder 1999)
5.52, 5.64 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

6.90*; 6.78 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
log K_{OA} = –6.30 + 3928/(T/K); temp range –10 to 20°C, ΔH_{OA} = 75.2 kJ/mol (Harner & Mackay 1995)
6.80 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
7.17, 6.90 (calculated-S_{oct} and vapor pressure P, quoted lit., Abraham et al. 2001)
7.384* (generator column-GC, measured range 5–25°C, Shoeib & Harner 2002)
7.38, 7.21 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.89 (rainbow trout, calculated-rate constant ratio k_1/k_2, Neely et al. 1974)
3.09 (fish, Körte et al. 1978)

4.27, 3.73, 4.34 (fathead minnow, rainbow trout, green sunfish, Veith et al. 1979b)
5.46 (guppy, lipid basis, Könemann & van Leeuwen 1980;)
4.27 (fish, Ciam et al. 1980)
1.20 (rats, adipose tissue, Geyer et al. 1980)
3.93, 2.46 (fish, flowing water, static water, Kenaga & Goring 1980; Kenaga 1980a)
4.39 (algae, Geyer et al. 1981)
3.38–4.08 mean 4.08; 3.88–4.30 mean 4.30 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
5.16–5.37 (15°C, rainbow trout, lipid basis, Oliver & Niimi 1983; quoted, Chiou 1985)
4.39, 3.36, 4.54 (algae, fish, activated sludge, Klein et al. 1984)
4.34 (sunfish; rainbow trout, 15°C, Davis & Dobbs 1984)
4.54 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
5.09 (green algae, dry wt basis, Geyer et al. 1985)
4.39, 3.41, 4.54 (algae, fish, activated sludge, Freitag et al. 1985)
2.62–2.97; 2.44–2.79 (human fat: lipid basis, wet weight, Geyer et al. 1987)
4.41 (algae, Mailhot 1987)
4.34 (fathead minnow, Carlson & Kosian 1987)
4.38, 4.30 (worms, fish, Oliver 1987a)
3.48 (fish-normalized, Tadokoro & Tomita 1987)
5.57, 5.62, 5.66, 5.76 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
6.42, 6.71, 5.96, 5.98 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
–1.35, –2.07, –0.32 (beef, milk, vegetable, reported as biotransfer factor log B_b, Travis & Arms 1988)
5.46 (guppy-lipid base, 12 to 31-d exposure studies, Gobas et al. 1989)
3.53 (*picea omorika*, Reischl et al. 1989)
3.57 (fish, calculated, Figueroa & Simmons 1991)
4.73; 4.76 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption; purge desorption, Koelmans et al. 1993)
3.74–4.30; 4.21; 4.34; 4.16; (*Oncorhynchus mykiss; Poecilia reticulata; Lepomis cyanellus; Oryzias latipes*, quoted lit., flow through conditions, Devillers et al. 1996)
5.62 (*Poecilia reticulata*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
3.18, 4.39 (macrophytes *Myrioophyllum spicatum*, algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)
5.55 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
4.38, 5.08 (algae *Chlorella*: wet wt basis, dry wt basis, Geyer et al.2000)
3.98, 5.98 (*Daphnia*: wet wt basis, lipid wt basis, Geyer et al.2000)
> 3.54, > 5.54 (mussel *Mytilus edulis* 21-d non-steady state: wet wt basis, lipid wt basis, Geyer et al.2000)
3.69, 5.71 (golden orfe *Leuciscus idus melanotus*, 0.95% lipid: wet wt basis, lipid wt basis, Geyer et al.2000)
2.65, 2.83 (human, fat: wet wt basis, lipid wt basis, Geyer et al.2000)
3.74; 3.95 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
3.59 (Kenaga & Goring 1980; Kenaga 1980a)
4.45 (Kenaga 1980a)
4.49 (soil, sorption isotherm, converted from reported log K_{OM} of 4.25, Briggs 1981)
2.56 (Speyer soil < 2.00 mm, Freundlich isotherm, Rippen et al. 1982)
2.70 (Alfisol, Freundlich isotherm, Rippen et al. 1982)
5.90; 5.50 (field data of Lake Ontario sediment trap material; Niagara River organic matter, Oliver & Charlton 1984)
4.90, 5.2–6.0 (bottom sediment, range, Karickhoff & Morris 1985)
5.2–6.7, 6.1; 5.80 (suspended sediment, average; algae > 50 µm, Oliver 1987c)
6.0–6.50, 6.30; 5.10 (Niagara River plume: range, mean; calculated-K_{OW}, Oliver 1987b)
4.77 (HPLC-k′ correlation, Hodson & Williams 1988)
4.66, 3.08, 4.91 (soil/water, soil-dextran/water, humic acid/water, batch equilibrium-sorption isotherm, Enfield et al. 1989)

3.23, 4.73; 4.59 (Captina silt loam OC 1.49%, McLaurie sandy loam OC 0.66%; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
5.51 (organic matter, Koelmans et al. 1993)
4.89 ± 0.36 (suspended particulates in coastal waters, Masunaga et al. 1996)
4.70; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
4.23, 3.79 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
5.53, 5.48 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:
4.25 (soil-organic matter, sorption isotherm, shake flask-GC, Briggs 1981)
5.50 (Niagara River-organic matter, Oliver & Charlton 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 3.45 \times 10^{-10}$ mol m^{-2} h^{-1} (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant in air, $k = 1.44 \times 10^{-2}$ h^{-1} (Brown et al. 1975; quoted, Mackay et al. 1985); photooxidation $t_{1/2}$ = 3753–37530 h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987).

Hydrolysis: not expected to be important, based on $k_h = 0$ was observed after 13 d at pH 3, 7, 11, and 85°C (Ellington et al. 1987, 1988).

Biodegradation: $t_{1/2}$(aq. aerobic) = 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974; Howard et al. 1991);
$t_{1/2}$(aq. anaerobic) = 93024–200544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974; Howard et al. 1991);
degradation rate constant $k = 1.9 \times 10^{-5}$ h^{-1} in soil (Beck & Hansen 1974; selected, Mackay et al. 1985; Mackay & Paterson 1991);
not significant in an aerobic environment, and no significant degradation rate (Tabak et al. 1981; Mills et al. 1982)
$t_{1/2}$(aerobic) = 970 d, $t_{1/2}$(anaerobic) = 3900 d in natural waters (Capel & Larson 1995)
dechlorination pseudo-first order rate constant $k = 0.282$ d^{-1} with $t_{1/2}$ = 2.5 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 18.76$ h^{-1}; $k_2 = 0.00238$ h^{-1} (trout muscle, Neely et al. 1974)
$k_1 = 10000$ d^{-1} (guppy, Könemann & van Leeuwen 1980)
$k_1 = 22.5$ h^{-1} (guppy, quoted from Konemann & van Leeuwen 1980, Hawker & Connell 1985)
log $k_1 = 1.35$ d^{-1} (fish, quoted from Konemann & Leeuwen 1980, Hawker & Connell 1985)
$k_1 = 18.8$ h^{-1} (trout, quoted from Bruggeman, Hawker & Connell 1985, Connell & Hawker 1988)
log $k_1 = 1.27$ d^{-1} (trout, quoted from Bruggeman, Hawker & Connell 1985, Connell & Hawker 1988)
$1/k_2 = 420$ h (trout, quoted from Bruggeman et al. 1984, Hawker & Connell 1985)
log $k_2 = 2.62$ d^{-1} (fish, quoted, Hawker & Connell 1985)
$k_1 = 540$ d^{-1} (fish, quoted, Opperhuizen 1986)
k_2 = 0.00510, 0.00818, 0.00640, 0.0047 d^{-1} (rainbow trout, calculated-fish mean body weight, Barber et al. 1988)
log $k_1 = 2.73$ d^{-1} (fish, quoted from Konemann & Leeuwen 1980, Connell & Hawker 1988)
log $k_1 = 2.65$ d^{-1}; log $1/k_2 = 1.24$ d (fish, quoted from Bruggeman et al. 1984, Connell & Hawker 1988)
log $k_2 = -1.24$ d^{-1} (fish, calculated-K_{OW}, Thomann 1989)
$k_1 = 0.049$ h^{-1}; $k_2 = 0.023$ h^{-1} (mayfly-sediment model II, Gobas et al. 1989b)
$k_2 = 0.092$ d^{-1} with elimination $t_{1/2}$ = 7.5 d (earthworm, Belfroid et al. 1995)
$k_1 = 6.558$ h^{-1}, $k_2 = 0.00429$ h^{-1} (Macrophytes *Myrioophyllum spicatum*, Wang et al. 1996)
$k_1 = 10489$ h^{-1}, $k_2 = 0.424$ h^{-1} (algae *Chlorella fusca*, Wang et al. 1996)
$k_2 = 0.016$ d^{-1} with $t_{1/2}$ = 43 d and $k_2 = 0.017$ d^{-1} with $t_{1/2}$ = 42 d for food concn of 14 ng/g and 103 ng/g respectively in a 30-d uptake followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_1 = 467$ mL g^{-1} d^{-1}, $k_2 = 0.26$ d^{-1} (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)
$k_1 = 8$ (food lipid mg)/(g worm lipid-d) (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 3753–37530 h, based on estimated photooxidation half-life (Atkinson 1987, Howard et al. 1991)
$t_{1/2}$ = 29 ± 5.8 yr at Eagle Harbor, $t_{1/2}$ = 15 ± 1.9 yr at Sleeping Bear Dunes and $t_{1/2}$ = 18 ± 2.3 yr in the Great Lakes = atmosphere at Sturgeon Point (Buehler et al. 2004).

Surface Water: $t_{1/2}$ = 1.4–50 d estimated, $t_{1/2}$ = 0.3–3 d for river water and $t_{1/2}$ = 30–300 d for lakes, estimated from persistence (Zoeteman et al. 1980)
$t_{1/2}$ = 23256–50136 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974, Howard et al. 1991)
$t_{1/2}$(aerobic) = 970 d, $t_{1/2}$(anaerobic) = 3900 d in natural waters (Capel & Larson 1995)

Groundwater: $t_{1/2}$ = 30–300 d, estimated from persistence (Zoeteman et al. 1980)
$t_{1/2}$ = 46512–100272 h, based on unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974, Howard et al. 1991)

Sediment: dechlorination $t_{1/2}$ = 1.8 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil: $t_{1/2}$ > 50 d (Ryan et al. 1988)
disappearance $t_{1/2}$ = 11.3 d from testing soils (Anderson et al. 1991)
$t_{1/2}$ = 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974; Howard et al. 1991)
$t_{1/2}$ = 3–6 yr in soil (Geyer et al. 2000)
$t_{1/2}$ = 48.7 and 11.7 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).

Biota: $t_{1/2}$ = 163 h, clearance from fish (Neely 1980)
$t_{1/2}$ > 224 d in rainbow trout (Niimi & Cho 1980);
$t_{1/2}$ = 210 d at 4°C, $t_{1/2}$ = 80 d at 12°C, $t_{1/2}$ = 70 d at 18°C in subadult rainbow trout (Niimi & Palazzo 1985)
$t_{1/2}$ = 27 d in worms at 8°C (Oliver 1987a)
biological $t_{1/2}$ = 12 d in trout muscle, $t_{1/2}$ > 173 d and > 224 d in trout, $t_{1/2}$ = 12 d in guppy (Niimi 1987);
$t_{1/2}$ = 30 d in *picea omorika* (Reischl et al. 1989)
elimination $t_{1/2}$ = 1.44 d and 12.3 d in a two-phase kinetics for earthworm in OECD soil (Belfroid et al. 1994)
elimination $t_{1/2}$ = 1.9–7.5 d from earthworm in soil (Belfroid et al. 1995)

Depuration $t_{1/2}$ = 42–43 d in a 30-d dietary exposure and 160-d duputation studies (juvenile rainbow trout, Fisk et al. 1998)

TABLE 6.1.1.12.1
Reported aqueous solubilities and Henry's law constants of hexachlorobenzene at various temperatures

Solubility						Henry's law constant	
OECD 1981		Shiu et al. 1997		Oleszek-Kudlak et al. 2004		Ten Hulscher et al. 1992	
gen. col./elution method		generator column-GC/ECD		generator column-GC/ECD		gas stripping-GC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	H/(Pa m³/mol)
15	0.00921†	5	0.0022	15	0.007	14.8	23.6
25	0.00996‡	15	0.0035	25	0.0096	20	41
		25	0.00544	25	0.010	20.1	30
†mean, 0.00206–0.0216 g/m³		35	0.00853	35	0.018	22.1	46.6
‡mean, 0.00119–0.0231 g/m³		45	0.014	45	0.024	24.1	52.5
				55	0.038	34.8	88.3
		ΔH_{sol} = 33.7 kJ/mol				50	217.2
				ΔH_{sol} = 33.5 kJ/mol			
						$\ln K_{AW} = A - B/(T/K)$	
						A	22.977
						B	5893.67

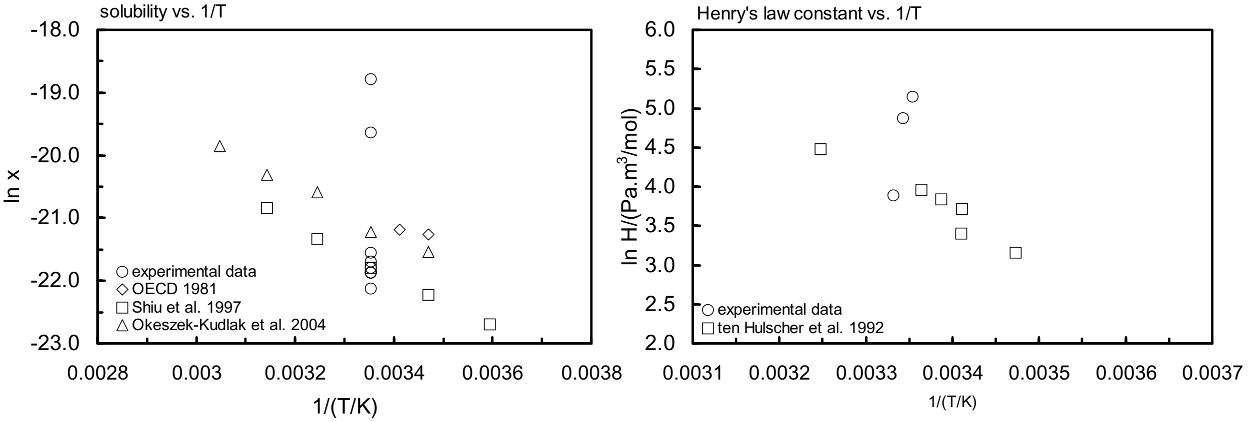


FIGURE 6.1.1.12.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for hexachlorobenzene.

TABLE 6.1.1.12.2
Reported vapor pressures of hexachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log (P/mmHg) = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log (P/Pa) = A - B/(C + T/K)$	(3)	$\ln (P/Pa) = A - B/(C + T/K)$	(3a)

1.

Stull 1947		Sears & Hopke 1949		Farmer et al. 1980		OECD 1981	
summary of lit. data		Rodebush gauge		gas saturation-GC		gas saturation/balance	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
114.1	133	measured 96–124°C		15	0.000528	10	0.0008
149.3	667			25	0.00255	20	0.0026
166.4	1333	eq. 1	P/mmHg	35	0.00853	30	0.0081
185.7	2666	A	11.397	45	0.0279	40	0.023
206	5333	B	4793.6	25	0.0023	50	0.081
219	7999					10	0.00028
235.5	13332			eq. 1	P/mmHg	20	0.0011
258.8	26664			A	12.94	30	0.003
283.5	53329			B	5279	40	0.013
309.4	101325					50	0.039
						eq. 1	P/mmHg
mp/°C	230					A	12.237
						B	5152.1

2.

Rordorf 1985		Liu & Dickhut 1994		Wania et al. 1994	
gas saturation		gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
41.05	0.0205	–15	2.21×10^{-6}	–30	2.567×10^{-6}
50.16	0.0547	–5.0	2.38×10^{-5}	–20	7.257×10^{-6}
60.3	0.165	10	2.62×10^{-4}	–10	3.229×10^{-5}

(Continued)

TABLE 6.1.1.11.2 *(Continued)*

Rordorf 1985		Liu & Dickhut 1994		Wania et al. 1994	
gas saturation		gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70.3	0.452	25	3.11×10^{-3}	0	1.03×10^{-4}
80.3	1.155	40	0.121	10	3.556×10^{-4}
90.4	2.77			20	1.092×10^{-3}
100.25	6.29	ΔH_V/(kJ mol^{-1}) = 81.3		30	3.276×10^{-3}
eq. 3	P/Pa	ΔH_{subl}/(kJ mol^{-1}) = 105		eq. 1	P/Pa
A	12.3243			A	10.83
B	4336.95			B	4044
C	–41.1905			ΔH_V/(kJ mol^{-1}) =: 77.4	

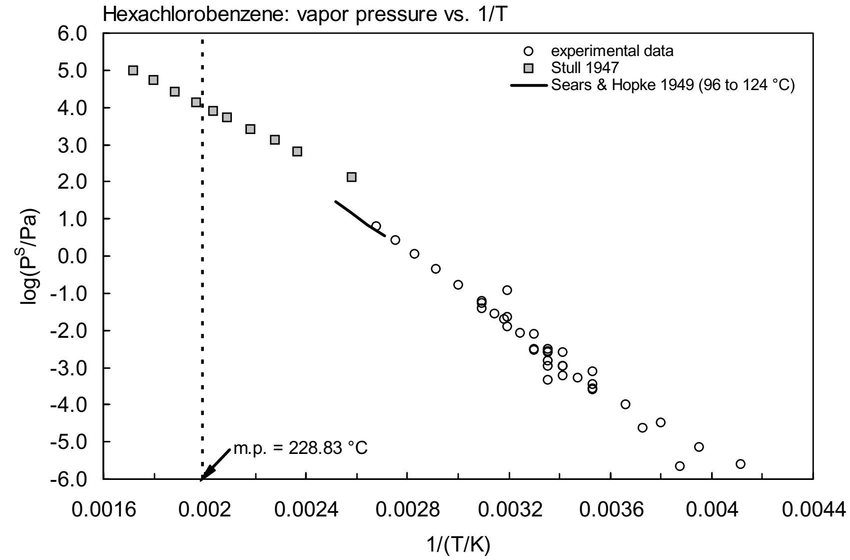


FIGURE 6.1.1.12.2 Logarithm of vapor pressure versus reciprocal temperature for hexachlorobenzene.

TABLE 6.1.1.12.3
Reported octanol-water partition coefficients and octanol-air partition coefficients of hexachlorobenzene at various temperatures

log K_{OW}				log K_{OA}			
Opperhuizen et al. 1988		**Bahadur et al. 1997**		**Harner & Mackay 1995**		**Shoeib & Harner 2002**	
shake flask-GC/ECD		**shake flask-GC/ECD**		**generator column-GC**			
t/°C	**log K_{OW}**	**t/°C**	**log K_{OW}**	**t/°C**	**log K_{OA}**	**t/°C**	**log K_{OA}**
13	5.68	5	5.74	25	6.9	5	8.1044
19	5.7	15	5.6	–10	8.653	10	7.887
28	5.58	25	5.46	0	8.105	15	7.7
33	4.66	35	5.3	10	6.213	20	7.5634
		45	5.17	18.5	7.185	25	7.3878
						25	7.384
$\Delta H/(kJ\ mol^{-1}) = -24.4$		enthalpy of transfer		$\Delta H_{OA}/(kJ\ mol^{-1}) = 75.2$		$\Delta H_{OA}/(kJ\ mol^{-1}) = 55.8$	
		$\Delta H/(kJ\ mol^{-1}) = -24.4$					
		$\log K_{OW} = A - \Delta H/2.303RT$		$\log K_{OA} = A + B/T$		$\log K_{OA} = A + B/T$	
		A	1.1806	A	–6.3	A	–2.395
		ΔH	–24400	B	3928	B	2914

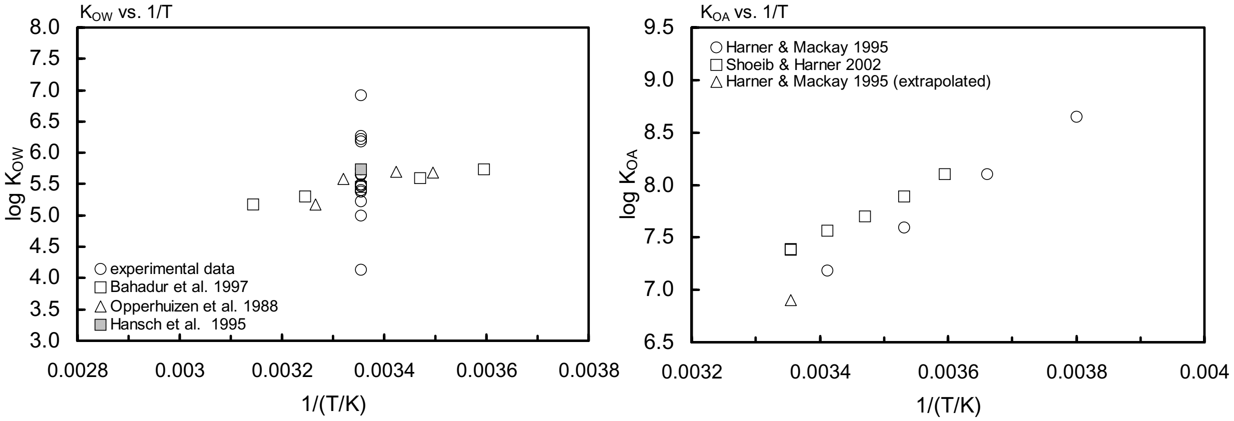
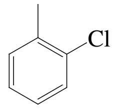


FIGURE 6.1.1.12.3 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for hexachlorobenzene.

6.1.2 CHLOROTOLUENES

6.1.2.1 2-Chlorotoluene



Common Name: 2-Chlorotoluene
Synonym: *o*-Tolylchloride, *o*-chlorotoluene, 2-chloro-1-methylbenzene
Chemical Name: 2-chlorotoluene
CAS Registry No: 95-49-8
Molecular Formula: C_7H_7Cl
Molecular Weight: 126.584
Melting Point (°C):
  –35.8 (Lide 2003)
Boiling Point (°C):
  159.15 (Dreisbach 1955; Weast 1982–83)
  159.0 (Dean 1985, 1992)
Density (g/cm^3 at 20°C):
  1.08245, 1.07762 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
Molar Volume (cm^3/mol):
  116.9 (20°C, calculated-density)
  139.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  8.368 (Dreisbach 1955; Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
  372 (Isnard & Lambert 1989)
  252.0 (shake flask, Fredenlund et al. 1995)
  117* ± 5.1 (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
  487 (interpolated-Antoine eq., Stuckey & Saylor 1940)
  log P/mmHg = 7.29547 – 1701.60/(T/K – 45.42); temp range 4–75°C (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)
  133.3*, 666.6, 1333 (5.4, 30.6, 43.2°C, summary of lit. data, temp range 5.4–159°C, Stull 1947)
  482.5 (calculated by formula, Dreisbach 1955; quoted, Riddick et al. 1986, Howard 1993)
  log (P/mmHg) = 6.94763 – 1497.2/(209.0 + t/°C); temp range 65–220°C (Antoine eq. for liquid state, Dreisbach 1955)
  482.5 (extrapolated-Antoine eq., Weast 1972–73)
  log (P/mmHg) = (–0.2185 × 10279.3)/(T/K) + 8.091764; temp range 5.4–159.3°C (Antoine eq., Weast 1972–73)
  5721* (72.654°C, temp range 72.654–158.323°C, Cervenkova & Boublik 1982)
  473 (extrapolated-Antoine eq., Boublik et al. 1984)
  log (P/kPa) = 6.09563 – 1507.930/(t/°C + 209.846); temp range 72.5–158.3°C (Antoine eq., Boublik et al. 1984)
  485 (interpolated-Antoine eq., Dean 1985, 1992)
  log (P/mmHg) = 7.36797 – 1735.8/(t/°C + 230.0); temp range 0–65°C (Antoine eq., Dean 1985, 1992)
  log (P/mmHg) = 6.94763 – 1497.2/(t/°C + 209.0); temp range: 65–220°C (Antoine eq., Dean 1985, 1992)
  472.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{Pa}) = 6.07253 - 1497.2/(T/\text{K} - 64.15)$; temp range 338–493K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 33.2792 - 3.4099 \times 10^3/(T/\text{K}) - 8.6743 \cdot \log(T/\text{K}) + 6.8174 \times 10^{-10} \cdot (T/\text{K}) + 1.8987 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 237–656 K (Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

370*	(23°C, equilibrium cell-GC, measured range 1–23°C, Leighton & Calo 1981)

$\ln(k_H/\text{atm}) = 17.18 - 3545/(T/\text{K})$; temp range:1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

295	(20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 3.890 - 1409/(T/\text{K})$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

3.42	(shake flask, Leo et al. 1971, Hansch & Leo 1979, Hansch et al. 1995)
3.52	(HPLC-RT correlation, Könemann et al. 1979)
3.40	(HPLC-k′ correlation, Hanai et al. 1981)
3.59	(RP-HPLC-RT correlation, Edsforth 1986)
3.52	(recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

TABLE 6.1.2.1.1
Reported aqueous solubilities, vapor pressures and Henry's law constants of 2-chlorotoluene at various temperatures

Aqueous solubility		Vapor pressure				Henry's law constant	
Ma et al. 2001		Stull 1947		Cernenkova & Boublik 1982		Leighton & Calo 1981	
shake flask-GC		summary of lit. data				equilibrium cell-GC	
t/°C	S/g·m⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	Pa m³/mol
5	89.4	5.4	133	72.654	5721	1	159.4
15	97.1	30.6	666.6	81.522	8325	3	112
25	117	43.2	1333	88.657	13911	12.4	178.5
35	128	56	2666	94.646	16792	12.5	216.1
45	132	72	5333	99.758	20277	17.9	243.5
		81.8	7999	105.05	24559	19.1	319.7
		94.7	13332	110.613	29367	22.7	3223
		115	26664	115.995	34778	23	369.7
		137.1	53329	121.252	40719		
		159	101325	126.313	47579	ln (H/atm) = A – B/(T/K)	
				139.532	60191	A	17.18
		mp/°C	-	147.287	74587	B	3545
				155.689	93400		
				158.323	99991		
				bp/°C	158.849		

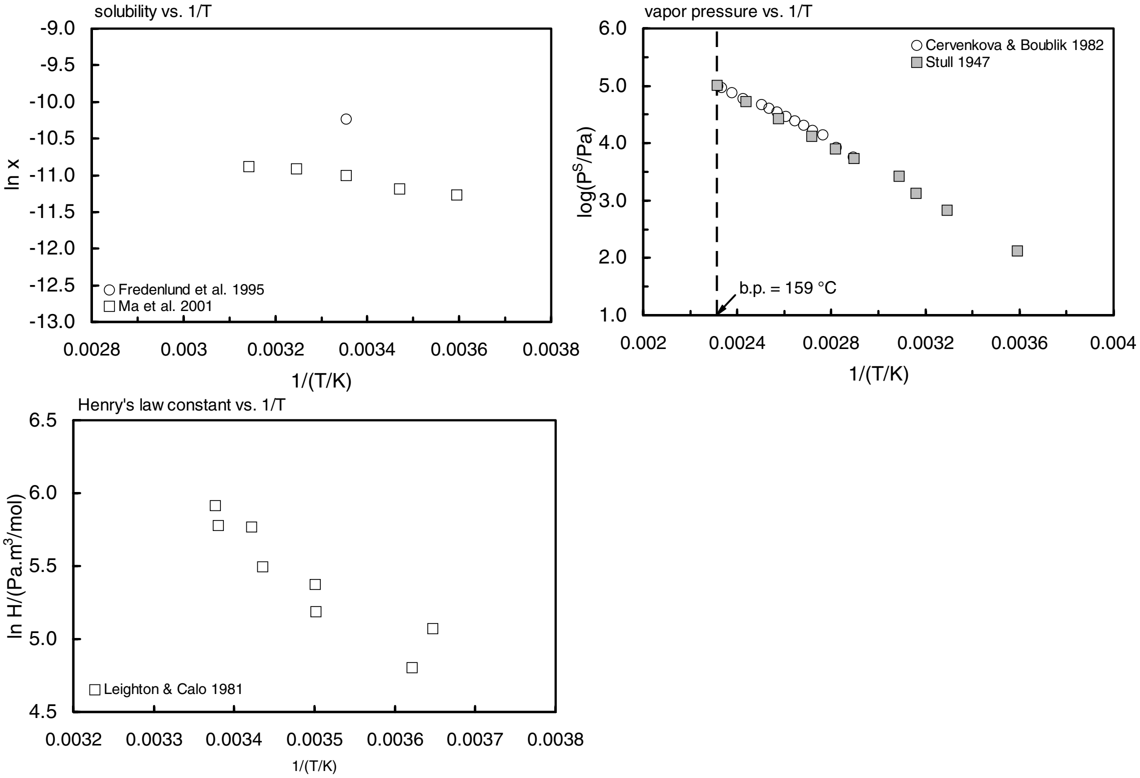
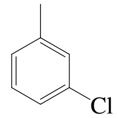


FIGURE 6.1.2.1.1 Logarithm of mole fraction solubility, vapor pressure and Henry's law constant versus reciprocal temperature for 2-chlorotoluene.

6.1.2.2 3-Chlorotoluene



Common Name: 3-Chlorotoluene
Synonym: *m*-Tolylchloride, 3-chloro-1-methylbenzene
Chemical Name: 3-chlorotoluene
CAS Registry No: 108-41-8
Molecular Formula: C_7H_7Cl
Molecular Weight: 126.584
Melting Point (°C):
 –47.8 (Weast 1982–83; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
 161.8 (Dean 1985; 1992; Lide 2003)
Density (g/cm^3 at 20°C):
 1.0722 (Weast 1982–83)
 1.0728 (20°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
 118.1 (20°C, calculated-density, Stephenson & Malanowski 1987)
 139.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 43.76 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
 372 (Isnard & Lambert 1989)
 117* ± 2.1 (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
 418 (interpolated-Antoine eq., Stuckey & Saylor 1940)
 log P/mmHg = 7.62515 – 1887.31/(T/K – 33.40); temp range 4–75°C (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)
 133.3*, 666.6, 1333 (4.8, 30.3, 43.2°C, summary of lit. data, temp range 4.8–162.3°C, Stull 1947)
 488.9 (extrapolated, Antoine eq., Weast 1972–73)
 log (P/mmHg) = (–0.2185 × 10081.1)/(T/K) + 7.952234; temp range 4.8–162.3°C (Antoine eq., Weast 1982–83)
 403.0 (extrapolated-Antoine eq., Boublik et al. 1984)
 log (P/kPa) = 6.09068 – 1511.858/(t/°C + 208.119); temp range 64.8–159.8°C (Antoine eq., Boublik et al. 1984)
 670.0 (Riddick et al. 1986)
 log (P/kPa) = 6.2794 – 1637.6/(223.3 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
 512.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 log (P/kPa) = 6.90317 – 2028.13/[(T/K) – 11.629]; temp range 277–436 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
 3.28 (shake flask, Leo et al. 1971, Hansch & Leo 1979)
 3.40 (HPLC-k′ correlation, Hanai et al. 1981)

3.28	(shake flask, Log P Database, Hansch & Leo 1987)
3.17	(calculated-UNFIC activity coefficients, Dallos et al. 1993)
3.28	(recommended, Sangster 1993)
3.28	(recommended, 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

3.88	(activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.2.2.1
Reported aqueous solubilities and vapor pressures of 3-chlorotoluene at various temperatures

Aqueous solubility		Vapor pressure	
Ma et al. 2001		Stull 1947	
shake flask-GC		summary of literature data	
t/°C	S/g·m^{-3}	t/°C	P/Pa
5	101	4.8	133
15	99.3	30.3	666.6
25	117	43.2	1333
35	113	57.4	2666
45	128	73	5333
		83.7	7999
		96.3	13332
		116.6	26664
		139.7	53329
		162.3	101325
		mp/°C	–

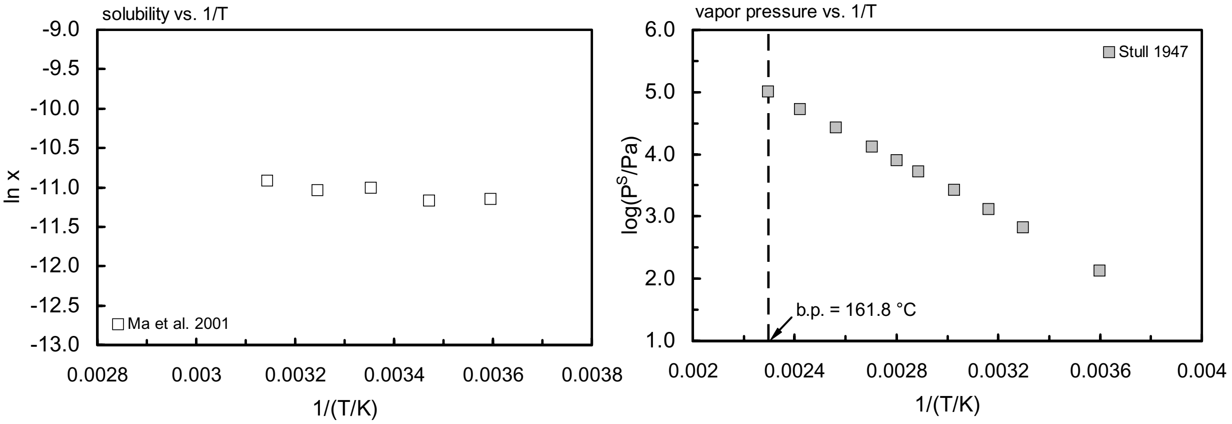
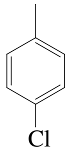


FIGURE 6.1.2.2.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 3-chlorotoluene.

6.1.2.3 4-Chlorotoluene



Common Name: 4-Chlorotoluene
Synonym: *p*-Tolylchloride, 4-chloro-1-methylbenzene
Chemical Name: 4-chlorotoluene
CAS Registry No: 106-43-4
Molecular Formula: C_7H_7Cl
Molecular Weight: 126.584
Melting Point (°C):
7.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
162.4 (Lide 2003)
Density (g/cm^3 at 20°C):
1.0697 (Weast 1982–83; Riddick et al. 1986; Dean 1985, 1992; Lide 2003)
Molar Volume (cm^3/mol):
118.3 (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
139.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
106.0 (20°C, Yalkowsky 1987)
123* ± 6.1 (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
422 (interpolated-Antoine eq., Stuckey & Saylor 1940)
$\log P/\text{mmHg} = 23.07210 - 3041.02/(T/K) - 5\cdot\log(T/K)$; temp range 4–75°C (vapor pressure eq. based on exptl. data, Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)
133.3*, 666.6, 1333 (5.5, 31.0, 43.8°C, temp range 5.5–162.3°C, summary of lit. data, Stull 1947)
471.6 (interpolated, Antoine eq., Weast 1982–83)
$\log(P/\text{mmHg}) = (-0.2185 \times 10151.7)/(T/K + 7.988366)$; temp range 5.5–162.3°C (Antoine eq., Weast 1982–83)
$\log(P/\text{kPa}) = 6.09068 - 1511.858/(t/°C + 208.199)$; temp range 65–160°C (Antoine eq., Boublik et al. 1984)
670 (30.3°C, Riddick et al. 1986)
$\log(P/\text{kPa}) = 6.75005 - 1887.31/(239.75 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)
506.7 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log(P/\text{kPa}) = 6.90317 - 2107.52/(T/K - 5.373)$; temp range 304–436 K (Antoine eq., Stephenson & Malanowski 1987)
$\log(P/\text{mmHg}) = 61.8901 - 4.3760 \times 10^3/(T/K) - 19.840\cdot\log(T/K) + 7.991 \times 10^{-3}\cdot(T/K) + 1.0781 \times 10^{-13}\cdot(T/K)^2$, temp range 281–660 K (Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
412.4 (calculated-P/C, Howard 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

3.33	(shake flask, Leo et al. 1971; Hansch & Leo 1979; 1985)
3.42	(HPLC-RT correlation, Könemann et al. 1979)
3.40	(HPLC-k′ correlation, Hanai et al. 1981)
3.30	(shake flask, Wang et al. 1987)
3.33	(recommended, Sangster 1993)
3.33	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.65–2.30	(estimated from log K_{OW}, Lyman et al. 1990; Howard1993)

Sorption Partition Coefficient, log K_{OC}:

2.65–3.19	(estimated from log K_{OW}, Lyman et al. 1990; Howard 1993)
4.10	(activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: based on the Henry's law constant, the volatilization $t_{1/2}$ ~ 3.5 h from a model river 1 m deep, flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: photooxidation $t_{1/2}$ = 8.4 d in the atmosphere with rate constant $k = 1.9 \times 10^{-12}$ $cm^3/molecule \cdot s$ at 25°C for the reaction with photochemically produced hydroxyl radicals (Atkinson 1987; quoted, Howard 1993).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 8.4 d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Atkinson 1987; quoted, Howard 1993).

Surface water: $t_{1/2}$ = 1.2 d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

TABLE 6.1.2.3.1
Reported aqueous solubilities and vapor pressures of 4-chlorotolune at various temperatures

Aqueous solubility		Vapor pressure			
Ma et al. 2001		Stull 1947		Cervenkova & Boublik 1982	
shake flask-GC		summary of lit. data			
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
5	99	5.50	133	64.855	3584
15	103	31.0	666.6	75.304	5727
25	123	43.8	1333	84.258	8333
35	136	57.8	2666	91.408	11078
45	153	73.5	5333	97.416	13924
		83.2	7999	102.574	16819
		96.6	13332	107.91	20322
		117.1	26664	113.464	24580
		139.8	53329	118.857	29380
		162.3	101325	124.14	34794
				129.212	40761
		mp/°C	7.3	134.395	47661
				142.507	60218
				150.285	74704
				158.718	93384
				159.801	96011
				bp/°C	161.904

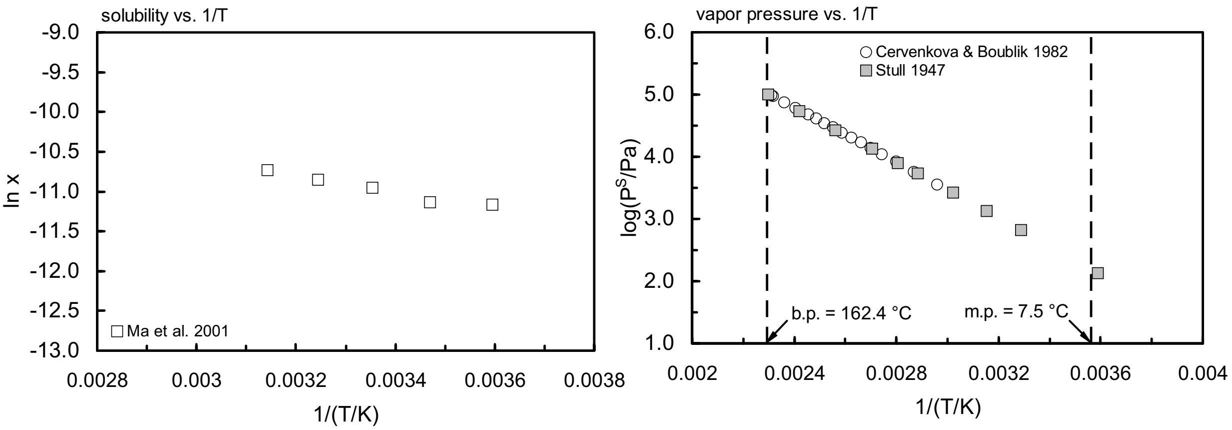
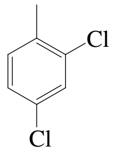


FIGURE 6.1.2.3.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 4-chlorotoluene.

6.1.2.4 2,4-Dichlorotoluene



Common Name: 2, 4-Dichlorotoluene
Synonym: 2, 4-dichloro-1-methylbenzene
Chemical Name: 2, 4-dichlorotoluene
CAS Registry No: 95-73-8
Molecular Formula: $C_7H_6Cl_2$
Molecular Weight: 161.029
Melting Point (°C):

–13.5	(Weast 1982–83, Lide 2003)

Boiling Point (°C):

201	(Lide 2003)

Density (g/cm^3 at 20°C):

1.2498	(Weast 1982–83)
1.2476	(Riddick et al. 1986, Lide 2003)
1.246	(Dean 1985, 1992)

Molar Volume (cm^3/mol):

128.6	(calculated-density, Stephenson & Malanowski 1987)
160.0	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
26.20 ± 2.1 (shake flask-GC/FID, Ma et al. 2001)
18.9, 26.2, 30.7, 37 (15, 25, 35, 45°C, shake flask-GC, Ma et al. 2001)
25.9 ± 2.2 (generator column-GC/FID, Ma et al. 2001)
22.3, 23.1, 25.9, 32, 36.6 (5, 15, 25, 35, 45°C, generator column-GC, Ma et al. 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
55.5 (Riddick et al. 1986)
$\log (P/kPa) = 5.6199 - 1330.4/(t/°C + 168.5)$ (Antoine eq., Riddick et al. 1986)
55.51 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 5.6199 - 1330.4/(T/K - 104.65)$; temp range 346–475 K (Antoine eq., Stephenson & Malanowski 1987)
61.06 (Daubert & Danner 1989)
$\log (P/mmHg) = 31.9325 - 3.7438 \times 10^3/(T/K) - 8.0123\cdot\log (T/K) - 7.5077 \times 10^{-11}\cdot(T/K) + 1.250 \times 10^{-6}\cdot(T/K)^2$, temp range 260–705 K (Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

350.6	(calculated, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:

4.24	(HPLC-RT correlation, Könemann et al. 1979)
4.24	(recommended, Sangster 1993)
4.24	(shake flask, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.99	(estimated from log K_{OW}, Howard 1997)

Sorption Partition Coefficient, log K_{OC}:

3.68	(estimated from log K_{OW}, Howard 1997)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 4.0 h in a model river 1-m deep with a 1 m/s current and a 3 m/s wind, $t_{½}$ = 1 d in the Rhine River in the Netherlands (Howard 1997)

Photolysis:

Oxidation: photooxidation $t_{½}$ = 11.6 d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

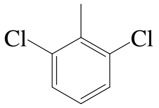
Half-Lives in the Environment:

Air: $t_{½}$ = 11.6 d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

Surface water: $t_{½}$ = 1.0 d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

volatilization $t_{½}$ = 4 h in a model river, $t_{½}$ = 1 d in Rhine River in the Netherlands (Howard 1993)

6.1.2.5 2,6-Dichlorotoluene



Common Name: 2, 6-Dichlorotoluene
Synonym:
Chemical Name: 2, 6-dichlorotoluene
CAS Registry No: 118-69-4
Molecular Formula: $C_7H_6Cl_2$
Molecular Weight: 161.029
Melting Point (°C): liquid
25.8 (Lide 2003)
Boiling Point (°C):
198 (Weast 1982–83, Lide 2003)
Density (g/cm^3 at 20°C):
1.254 (Dean 1992)
1.2686 (Lide 2003)
Molar Volume (cm^3/mol):
126.9 (20°C, calculated-density)
160.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
23.3 ± 0.81 (shake flask-GC/FID, Ma et al. 2001)
16.7, 19.8, 23.3, 30.1, 33 (5, 15, 25, 35, 45°C, shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at 25°C):
53.19 (estimated, Lyman et al. 1990, Howard 1997)

Henry's Law Constant (Pa·m^3/mol):
350.6 (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:
4.29 (HPLC-k′ correlation, Könemann et al. 1979)
4.29 (recommended, Sangster 1983)
4.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
3.03 (estimated from log K_{OW}, Howard 1997)

Sorption Partition Coefficient, log K_{OC}:
3.71 (estimated from log K_{OW}, Howard 1997)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:
Volatilization: based on Henry's law constant, an estimated $t_{1/2}$ = 4.0 h of volatilization from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Howard 1997).
Photolysis:

Oxidation: photooxidation $t_{1/2}$ = 11.6 d in the atmosphere for reaction with photochemically produced hydroxyl radical (Howard 1997).

Hydrolysis:

Biodegradation:

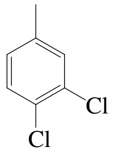
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 11.6 d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

6.1.2.6 3,4-Dichlorotoluene



Common Name: 3, 4-Dichlorotoluene
Synonym: 3, 4-dichloro-1-methylbenzene
Chemical Name:
CAS Registry No: 95-75-0
Molecular Formula: $C_7H_6Cl_2$
Molecular Weight: 161.029
Melting Point (°C):
–15.2 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
208.9 (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.25256, 1.24751 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
1.2564 (Weast 1982–83; Lide 2003)
Molar Volume (cm^3/mol):
127.9 (calculated-density, Stephenson & Malanowski 1987)
160.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
13.33, 10.13 (25°C, bp, Dreisbach 1955; Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
10.544 (Dreisbach 1955)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
26 (30°C, Dreisbach 1955; IUPAC Solubility Data Series, Horvath & Getzen 1985; Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
42 (calculated by formula, Dreisbach 1955)
$\log (P/mmHg) = 6.97925 - 1655.4/(195.0 + t/°C)$; temp range 105–270°C (Antoine eq. for liquid state, Dreisbach 1955)
$\log (P/mmHg) = 6.91048 - 946.35/(246.68 + t/°C)$; temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
42.0 (Riddick et al. 1986)
$\log (P/kPa) = 6.10415 - 1655.44/(195.0 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)
$\log (P_L/kPa) = 6.10415 - 1655.4/(T/K - 78.15)$; temp range 378–543 K (Antoine eq., Stephenson & Malanowski 1987)

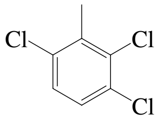
Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
4.067 (Verhaar et al. 1992)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Half-Lives in the Environment:

6.1.2.7 2,3,6-Trichlorotoluene



Common Name: 2, 3, 6-Trichlorotoluene
Synonym:
Chemical Name: 2, 3, 6-trichlorotoluene
CAS Registry No: 2077-46-5
Molecular Formula: $C_7H_5Cl_3$
Molecular Weight: 195.474
Melting Point (°C):
45–46 (Weast 1982–83)
Boiling Point (°C):
229.5 (Weast 1982–83)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
180.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.629 (mp at 45.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.08 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 5.6249 - 1323/(T/\text{K} - 144.15)$; temp range 384–509 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
152 (gas stripping-GC, Oliver 1985)
245 (calculated-bond contribution method, Meylan & Howard 1991)

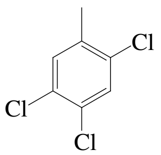
Octanol/Water Partition Coefficient, log K_{OW}:
4.80 (calculated as per Hansch & Leo 1979, Oliver 1987b)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:
Biota: elimination $t_{½} < 5$ d, observed and corrected for growth dilution in oligochaete worms (Oliver 1987b)

6.1.2.8 2,4,5-Trichlorotoluene



Common Name: 2, 4, 5-Trichlorotoluene
Synonym: 2, 4, 5-TCT
Chemical Name: 2, 4, 5-trichlorotoluene
CAS Registry No: 6639-30-1
Molecular Formula: $C_7H_5Cl_3$
Molecular Weight: 195.474
Melting Point (°C):

82.4	(Weast 1982–83; Lide 2003)

Boiling Point (°C):

231	(Lide 2003)

Density (g/cm^3 at 20°C):

1.1004	(Lide 2003)

Molar Volume (cm^3/mol):

115.0	(20°C, calculated-density)
180.9	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.273 (mp at 82.4°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
2.33 ± 0.22 (shake flask-GC/FID, Ma et al. 2001)
1.10, 1.38, 2.33, 3.33, 5.64 (5, 15, 25, 35, 45°C, shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

152	(gas stripping-GC, Oliver 1985)

Octanol/Water Partition Coefficient, log K_{OW}:

4.82	(calculated-π method of Hansch & Leo 1979, Oliver & Niimi 1984, 1985)
4.80	(Oliver & Niimi 1985)
4.780	(Verhaar et al. 1992)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
3.68 (rainbow trout, Oliver & Niimi 1984; Oliver 1987)
3.54–3.99 with mean value of 3.88; 3.52–4.04 with mean value of 3.93 (rainbow trout, wet wt., 15°C, steady-state BCF on 7- to 96-d laboratory study on two tanks of different water concn, Oliver & Niimi 1985)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ = 1.8 d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

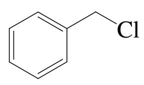
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} < 5$ d, observed and corrected for growth dilution in oligochaete worms (Oliver 1987b).

6.1.2.9 α-Chlorotoluene



Common Name: α-Chlorotoluene
Synonym: chloromethylbenzene, benzyl chloride
Chemical Name:
CAS Registry No: 100-44-7
Molecular Formula: C_7H_7Cl, $C_6H_5CH_2Cl$
Molecular Weight: 126.584
Melting Point (°C):
–45 (Lide 2003)
Boiling Point (°C):
179 (Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
118.0 (calculated-density, Stephenson & Malanowski 1987)
139.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
493 (20°C, Riddick et al. 1986)
579 (calculated-fragment const., Wakita et al. 1986)
236 (calculated-group contribution, Kühne et al. 1995)
409 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (22.0°C, summary of lit. data, Stull 1947)
$\log(P/\text{mmHg}) = [-0.2185 \times 11158.7/(T/K)] + 8.290189$; temp range 22–179.4°C (Antoine eq., Weast 1972–73)
641* (47.84°C, isoteniscope method, measured range 47.84–117.08°C, Ashcroft 1976)
$\log(P/\text{mmHg}) = 6.801 - 1477/(216.9 + t/°C)$; temp range 48–117°C (isoteniscope method, Ashdroft 1976)
641 (Riddick et al. 1986)
$\log(P/\text{kPa}) = 5.926 - 1477/(193.7 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)
170 (interpolated-Anotine eq., Stephenson & Malanowski 1987)
$\log(P/\text{kPa}) = 6.7176 - 1954.13/(T/K - 38.02)$; temp range 295–453 K (Antoine eq., Stephenson & Malanowski 1987)
$\log(P/\text{kPa}) = 7.73903 - 2642.08/(T/K + 12.819)$; temp range 320–390 K (Antoine eq., Stephenson & Malanowski 1987)
$\log(P/\text{mmHg}) = 12.1503 - 2.9139 \times 10^3/(T/K) - 0.3712 \cdot \log(T/K) - 5.2889 \times 10^{-3} \cdot (T/K) + 2.6296 \times 10^{-6} \cdot (T/K)^2$, temp range 234–686 K (Yaws 1994)
133.05* (24.05°C, transpiration method, measured range 276–309 K, Krasnykh et al. 2002)
$\ln(P/\text{Pa}) = 281.417/R - 71588.799/R(T/K) - (72.0/R) \cdot \ln[(T/K)/298.15]$; temp range 276–309 K (transpiration method, Krasnykh et al. 2002)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
159.4, 122, 178, 216, 243.5, 320, 322, 370 (1.0, 3.0, 12.4, 12.5, 17.9, 19.1, 22.7, 23.0°C, equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
$\ln(k_H/\text{atm}) = 17.18 - 3545/(T/K)$; temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
36.07 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O3} < 0.04 \times 10^{-18}$ cm³ molecule⁻¹ s⁻¹ at 296 K with a tropospheric lifetimes $\tau > 290$ d and $\tau \sim 3$ d due to reactions with O_3 and OH radical at room temp. (Atkinson et al. 1982)

$k_{OH} = (2.95 \pm 0.15) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with a atmospheric lifetime $\tau = 3.9$ d at room temp. (relative rate method, Edney et al. 1986)

k_{OH}(calc) $= 2.1 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, k_{OH}(obs) $= 2.9 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = 2.90 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

$t_{½}$ = 22–218 h, based on photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: rate constant $k = 1.28 \times 10^{-5}$ s⁻¹ and $t_{½}$ = 15 h at 25°C and pH 7 (Mabey & Mill 1978)

neutral rate constant $k = 8.5 \pm 0.5$ min⁻¹ at 25°C (Ellington et al. 1988)

$t_{½}$ = 25–290 h based on overall hydrolysis rate constant (Howard et al. 1991)

Biodegradation: $t_{½}$(aerobic) = 168–672 h, based on unacclimated aqueous screening test data; $t_{½}$(anaerobic) = 672–2688 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetimes $\tau > 290$ d and $\tau \sim 3$ d due to reactions with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982);

calculated atmospheric lifetime $\tau = 3.9$ d due to reaction with OH radical at room temp. (Edney et al. 1986)

$t_{½}$ = 22–218 h, based on photooxidation half-life in air (Howard et al. 1991)

Surface water: $t_{½}$ = 15–290 h, based on estimated hydrolysis half-lives (Howard et al. 1991)

Groundwater: $t_{½}$ = 15–290 h, based on estimated hydrolysis half-lives (Howard et al. 1991)

Sediment:

Soil: $t_{½}$ = 15–290 h, based on estimated hydrolysis half-lives (Howard et al. 1991)

Biota:

TABLE 6.1.2.9.1
Reported vapor pressures of a-chlorotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log (P/\text{mmHg}) = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$ (3)
$\log (P/\text{mmHg}) = A - B/(T/K) - C\cdot\log (T/K)$ (4)

Stull 1947		Ashcroft 1976		Krasnykh et al. 2002	
summary of lit. data		isoteniscope method		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
22.0	133	47.84	641.3	2.85	26.95
47.8	666.6	53.37	905.3	4.85	32.31
60.8	1333	70.60	2177	6.85	38.60

(Continued)

TABLE 6.1.2.9.1 (*Continued*)

Stull 1947		Ashcroft 1976		Krasnykh et al. 2002	
summary of lit. data		isoteniscope method		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
75.0	2666	85.63	4246	8.85	43.78
90.7	5333	95.35	6330	10.85	51.48
100.5	7999	100.2	7905	12.85	60.14
114.2	13332	106.95	10566	12.95	60.61
134.0	26664	122.67	12883	13.95	64.27
1558	53329	117.08	17857	14.95	70.50
179.4	101325			15.95	75.36
		eq. 2	P/mmHg	17.95	98.72
mp/°C	–39	A	6.801	18.95	97.84
		B	1477	20.05	101.6
		C	193.7	21.15	111.0
				22.05	117.44
		ΔH_V(kJ mol^{-1}) = 50.1		24.05	133.06
			at 25°C	26.05	153.53
				28.15	175.98
				30.15	204.90
				32.15	232.87
				34.15	257.42
				36.15	295.82
				ΔH_V(kJ mol^{-1}) = 50.12	
					at 25°C

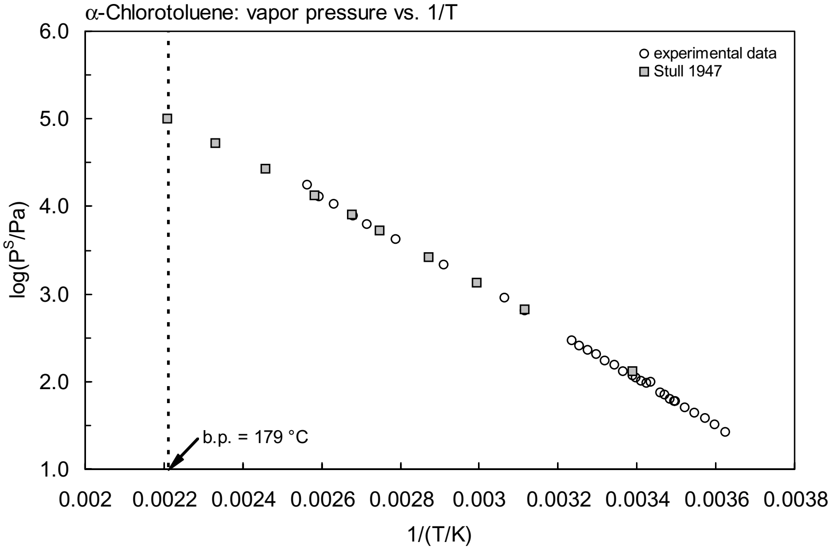
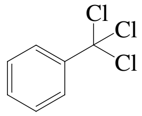


FIGURE 6.1.2.9.1 Logarithm of vapor pressure versus reciprocal temperature for α-chlorotoluene.

6.1.2.10 α, α, α-Trichlorotoluene



Common Name: α, α, α-Trichlorotoluene
Synonym: trichloromethylbenzene, benzotrichloride
Chemical Name: α, α, α-Trichlorotoluene
CAS Registry No: 98-07-7
Molecular Formula: $C_7H_5Cl_3$, $C_6H_5CCl_3$
Molecular Weight: 195.474
Melting Point (°C):
–4.42 (Lide 2003)
Boiling Point (°C):
221 (Lide 2003)
Density (g/cm^3 at 20°C):
1.3723 (20°C, Lide 2003)
Molar Volume (cm^3/mol):
142.4 (20°C, calculated-density, Stephenson & Malanowski 1987)
180.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
5.30 (5°C, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (45.8, summary of lit. data, Stull 1947)
$\log(P/\text{mmHg}) = [-0.2185 \times 8869.7/(T/K)] + 8.071972$, temp range 32–102.2°C (Antoine eq., Weast 1972–73)
34.67 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
$\log(P_L/\text{kPa}) = 6.95923 - 2268.82/(T/K - 28.669)$; temp range 318–487 K (Antoine eq., Stephenson & Malanowski 1987)
$\log(P/\text{mmHg}) = 0.4912 - 2.7285 \times 10^3/(T/K) + 4.4706 \cdot \log(T/K) - 1.058 \times 10^{-2} \cdot (T/K) + 4.7621 \times 10^{-6} \cdot (T/K)^2$; temp range 268–737 K (Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
2.92 (shake flask, Leo et al. 1979, Hansch & Leo 1979, Hansch et al. 1995; quoted, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: $t_{1/2}$ = 173.7–1737 h, based on photooxidation half-life in air (Howard et al. 1991)
Hydrolysis: rate constant $k = 6.3 \times 10^{-2}\ s^{-1}$ and $t_{1/2}$ = 19 s at 25°C and pH 7 (Mabey & Mill 1978)
$t_{1/2}$ = 11 s – 3 min, based on overall hydrolysis rate constants (Howard et al. 1991)

Biodegradation: $t_{½}$(aerobic) = 24–168 h, based on limited aqueous screening test data; $t_{½}$ = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

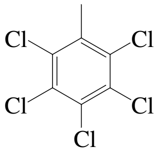
Half-Lives in the Environment:

Air: $t_{½}$ = 173.7–1737 h, based on photooxidation half-life in air (Howard et al. 1991)
Surface water: $t_{½}$ = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)
Groundwater: $t_{½}$ = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)
Sediment:
Soil: $t_{½}$ = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)
Biota:

TABLE 6.1.2.10.1
Reported vapor pressures of α, α, α-chlorotoluene at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
45.8	133.3
73.7	666.6
87.6	1333
102.7	2666
119.8	5333
130.0	7999
144.3	13332
165.6	26664
189.2	53329
213.5	101325
mp/°C	–21.2

6.1.2.11 Pentachlorotoluene



Common Name: Pentachlorotoluene
Synonym:
Chemical Name: pentachlorotoluene
CAS Registry No: 877-11-1
Molecular Formula: $C_7H_3Cl_5$
Molecular Weight: 264.364
Melting Point (°C):
224.8 (Lide 2003)
Boiling Point (°C):
301 (Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
222.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.011 (mp at 224.8°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.028 ± 0.001, 0.047 ± 0.004 (25, 35°C, shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
6.20 (calculated as per Hansch & Leo 1979, Oliver & Niimi 1985; Oliver 1987b)
5.50 (assumed to have approx. the same K_{OW} of HCB, Oliver & Charlton 1984)

Octanol/Air Partition Coefficient, log K_{OA}:

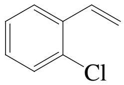
Bioconcentration Factor, log BCF at 25°C or as indicated:
3.38–3.86 mean 3.83 (rainbow trout, wet wt., 15°C, steady-state BCF, 7- to 96-d laboratory study, Oliver & Niimi 1985)
3.83; 4.36 (rainbow trout, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)
4.45; 3.83 (oligochaete worm; fish, Oliver 1987b)

Sorption Partition Coefficient, log K_{OC}:
5.30 (field data of sediment trap material; Oliver & Charlton 1984)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Half-Lives in the Environment:
Biota: elimination $t_{½}$ = 22 and 26 d, observed and corrected for growth dilution, respectively, in oligochaete worms (Oliver 1987b)

6.1.2.12 *o*-Chlorostyrene



Common Name: *o*-Chlorostyrene
Synonym: *o*-chlorovinylbenzene, 2-chlorostyrene
Chemical Name: *o*-chlorostyrene
CAS Registry No: 2039-87-4
Molecular Formula: C_8H_7Cl
Molecular Weight: 138.595
Melting Point (°C):
    –63.1 (Lide 2003)
Boiling Point (°C):
    188.7 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3):
    1.10001, 1.09532 (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm^3/mol):
    126.0 (20°C, calculated-density, Stephenson & Malanowski 1987)
    153.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    51.03, 40.01 (25°C, bp, Dreisbach 1955)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

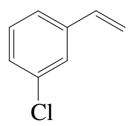
Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    127.5 (calculated by formula, Dreisbach 1955)
    $\log (P/mmHg) = 6.86644 - 1542.1/(198 + t/°C)$; temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)
    $\log (P/kPa) = 6.11856 - 1627.284/(207.112 + t/°C)$; temp range 98.5–154.9°C (Antoine eq. derived from experimental data of Dreisbach & Shrader 1949, Boublik et al. 1984)
    $\log (P_L/kPa) = 5.99134 - 1541.1/(-75.15 + T/K)$; temp range 363–543 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:

6.1.2.13 *m*-Chlorostyrene



Common Name: *m*-Chlorostyrene
Synonym: *m*-chlorovinylbenzene, 3-chlorostyrene
Chemical Name: *m*-chlorostyrene
CAS Registry No: 2039-85-2
Molecular Formula: C_8H_7Cl
Molecular Weight: 138.595
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):

1.1033	(20°C, Lide 2003)

Molar Volume (cm^3/mol):

124.1	(20°C, calculated-density, Stephenson & Malanowski 1987)
153.9	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3*	(25.3°C, summary of literature data, Stull 1947)
148.06	(interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.83847 - 2156.77/(-16.882 + T/K)$; temp range 298–463 K (Antoine eq., Stephenson & Malanowski 1987)

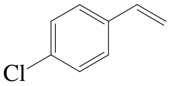
Henry's Law Constant (Pa m^3/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant, k, and Half-Lives, $t_{½}$:
Half-Lives in the Environment:

TABLE 6.1.2.13.1
Reported vapor pressures of m-chlorostyrene at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
25.3	133.3
51.3	666.6
65.2	1333
80.0	2666
96.5	5333
107.2	7999
121.1	13332
142	26664
165.7	53329
190	101325

6.1.2.14 *p*-Chlorostyrene



Common Name: *p*-Chlorostyrene
Synonym: *p*-chlorovinylbenzene, 4-chlorostyrene
Chemical Name: *p*-chlorostyrene
CAS Registry No: 1073-67-2
Molecular Formula: C_8H_7Cl
Molecular Weight: 138.595
Melting Point (°C):
–15.9 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
192.0 (Dreisbach 1955, Lide 2003)
Density (g/cm^3):
1.08682, 1.08214 (20°C, 25°C, Dreisbach 1955)
1.0868 (20°C, Lide 2003)
Molar Volume (cm^3/mol):
127.5 (20°C, calculated-density, Stephenson & Malanowski 1987)
153.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
51.11, 40.07 (25°C, bp, Dreisbach 1955)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (28.0°C, summary of literature data, temp range 28.0–191.0°C, Stull 1947)
6287* (100.91°C, ebulliometry, measured range 100.91–127.27°C, Dreisbach & Shrader 1949)
116.3 (calculated by formula, Dreisbach 1955)
$\log (P/mmHg) = 6.84248 - 1545.0/(198 + t/°C)$; temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)
$\log (P/kPa) = 9.18404 - 4186.871/(398.256 + t/°C)$; temp range 100.9–127.27°C (Antoine eq. derived from experimental data of Dreisbach & Shrader 1949, Boublik et al. 1984)
$\log (P_L/kPa) = 5.96738 - 1545.0(-75.15 + T/K)$; temp range 363–523 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
3.66 (estimated, Kaiser 1987)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant, k, and Half-Lives, $t_{½}$:
Half-Lives in the Environment:

TABLE 6.1.2.14.1
Reported vapor pressures of *p*-chlorostyrene at various temperatures

Stull 1947		Dreisbach & Shrader 1949	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
28.0	133.3	100.91	6287
54.5	666.6	106.09	7605
67.5	1333	109.97	8851
82.0	2666	113.76	10114
98.0	5333	127.27	16500
105.8	7999		
122.0	13332		
143.5	26664		
166.0	53329		
191.0	101325		

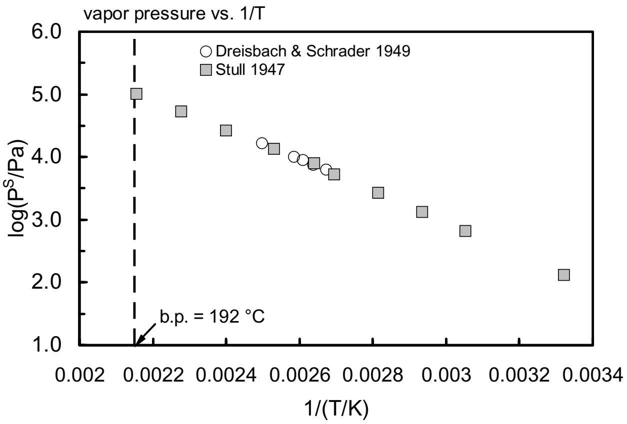
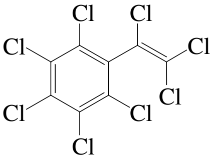


FIGURE 6.1.2.14.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-chlorostyrene.

6.1.2.15 Octochlorostyrene



Common Name: Octochlorostyrene
Synonym:
Chemical Name: octachlorostyrene
CAS Registry No: 29082-74-4
Molecular Formula: C_8Cl_8
Molecular Weight: 379.710
Melting Point (°C):
  99 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  300.2 (calculated-Le Bas method at normal boiling point0
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.188 (mp at 99°C)

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):
  22.9(20°C, calculated-bond contribution method, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
  6.29 (HPLC-RT correlation, Veith et al.1979b)
  6.20 (HPLC-RT correlation, Veith et al. 1979a)

Bioconcentration Factor, log BCF:
  4.52 (fathead minnow, 32-d exposure, Veith et al. 1979b)
  2.91–3.91, mean 3.91 (rainbow trout, 15°C, wet wt., steady-state BCF on 7- to 96-d laboratory study; Oliver & Niimi 1985)
  5.38; 6.15 (rainbow trout, calculated-K_{OW}, Lake Ontario field BCF, Oliver & Niimi 1985)
  4.49; 3.91 (oligochaete worms; fish, Oliver 1987b)

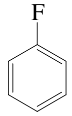
Sorption Partition Coefficient, log K_{OC}:
  6.10 (field data of sediment trap material, Oliver & Charlton 1984)
  5.90–7.30; 6.60 (suspended sediment: range; mean, Oliver 1987a)
  6.30 (algae > 50 μm, mean, Oliver 1987a)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:
  Biota: elimination $t_{½}$ = 71 d, observed and $t_{½}$ = 100 d, corrected for growth dilution in worms (8°C, Oliver 1987).

6.1.3 FLUOROBENZENES

6.1.3.1 Fluorobenzene



Common Name: Fluorobenzene
Synonym: phenyl fluoride
Chemical Name: fluorobenzene, phenyl fluoride
CAS Registry No: 462-06-6
Molecular Formula: C_6H_5F
Molecular Weight: 96.102
Melting Point (°C):
–42.18 (Lide 2003)
Boiling Point (°C):
84.73 (Riddick et al. 1986; Lide 2003)
Density (g/cm^3 at 20°C):
1.0225 (Horvath 1982; Lide 2003)
1.0131 (30°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
94.4 (Stephenson & Malanowski 1987; Wang et al. 1992)
101.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.305 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1540 (30°C, shake flask-IR, Gross et al. 1933)
1550 (shake flask-UV spectrophotometer, Andrews & Keefer 1950)
1296 (Deno & Berkheimer 1960)
922 (shake flask-GC, Jones et al. 1977/1978)
189.3* (shake flask-GC, measured range 5–45°C, Nelson & Smit 1978)
1559 (Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
1540 (27.5°C, recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
1530 (30°C, Riddick et al. 1986)
1700*, 1550 (19.2°C, 29.7°C, shake flask-GC/TC, measured range 0–80°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
10246* (24.9°C, Ramsay-Young method, measured range –17.85 to 83.85°C, Young 1889)
7999* (19.6°C, summary of literature data, temp range –43.4 to 84.7°C, Stull 1947)
19920* (39.4°C, comparative ebulliometry, measured range 39.4–120.5°C, Scott et al. 1956)
$\log(P/mmHg) = 6.95208 - 1248.083/(221.827 + t/°C)$; temp range 34.5–120.5°C (Antoine eq., comparative ebulliometry, Scott et al. 1956)
$\log(P/mmHg) = [-0.2185 \times 7980.4/(T/K)] + 7.699237$; temp range –43.4–279.3°C (Antoine eq., Weast 1972–73)
10200 (interpolated-Antoine eq., Boublik et al. 1973, 1984)
$\log(P/mmHg) = 7.18703 - 1381.828/(235.563 + t/°C)$; temp range –17.85 to 83.85°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log(P/kPa) = 6.31155 - 1381.646/(235.548 + t/°C)$; temp range –17.85 to 83.85°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.1870 - 1381.8/(235.6 + t/°C)$; temp range –18 to 84°C (Antoine eq., Dean 1985, 1992)

10480	(Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.07698 - 1248.083/(221.827 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.07234 - 1245.564/(-51.587 + T/K)$; temp range 312–394 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.4113 - 1398.61/(-31.295 + T/K)$; temp range 358–530 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14135 - 1291.116/(-45.664 + T/K)$; temp range 373–419 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.37857 - 1478.807/(-18.847 + T/K)$; temp range 414–501 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.59182 - 2876.741/(171.093 + T/K)$; temp range 497–561 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -5.4849 - 1.8597 \times 10^3/(T/K) + 7.1515\cdot\log (T/K) - 1.6467 \times 10^{-2}\cdot(T/K) + 9.2622 \times 10^{-6}\cdot(T/K)^2$, temp range 231–560 K (Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

632	(computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.27	(shake flask-AS, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)
2.28	(calculated-fragment const., Rekker 1977)
2.27	(recommended, Sangster 1989, 1993)
2.26	(centrifugal partition chromatography, El Tayar et al.1991)
2.27	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}(\text{calc}) = 2.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{OH}(\text{obs}) = 0.54 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}{}^* = (6.31 \pm 0.84) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{OH} = 6.31 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}; k(soln) = 1.7×10^{-11} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{OH} = 6.90 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 234–303 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 1.08 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 6.1.3.1.1
Reported aqueous solubilities of fluorobenzene at various temperatures

Gross et al. 1933		Nelson & Smit 1978		Stephenson 1992	
shake flask-interferometer		shake flask-GC		shake flask-GC/TC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
30	1540	5	118.4	0	1620
		25	189.3	9.5	1660
		35	336	29.7	1700
		45	512	39.6	1530
Andrews & Keefer 1950				47.7	1730
shake flask-UV				60.1	1900
t/°C	**S/g·m^{-3}**			70	1901
25	1550			80	1880

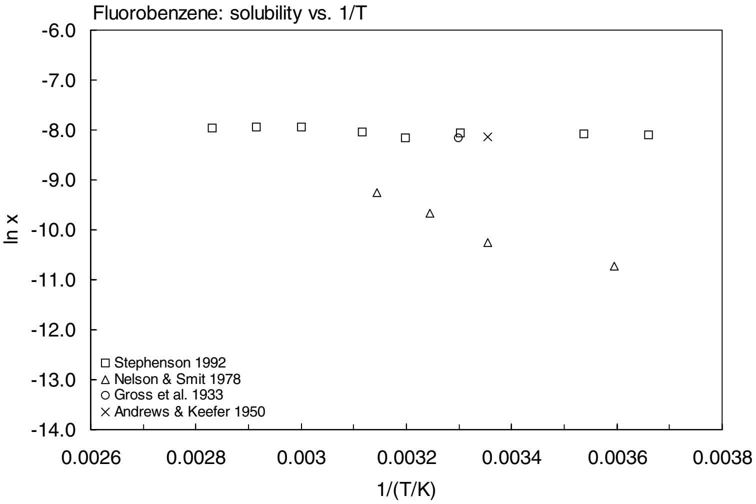


FIGURE 6.1.3.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for fluorobenzene.

TABLE 6.1.3.1.2
Reported vapor pressures of fluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Young 1889		Stull 1947		Scott et al. 1956	
Ramsay-Young method		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–17.85	927	–43.4	133.3	39.404	19920
–5.95	1980	–22.8	666.6	44.920	25007
0.15	2806	–12.4	1333	50.480	31160
4.7	3613	–1.20	2666	56.081	38567
10.65	5000	11.5	5333	61.726	47359
16.75	6873	19.6	7999	67.412	57803
19.5	7866	30.4	13332	73.141	70109
24.9	10246	47.2	26664	78.916	84525
30.35	12999	65.7	53329	84.734	101325
36.05	16759	84.7	101325	90.590	120798
42.05	21558			96.497	143268
49.6	29317	mp/°C	–42.1	102.438	169-53
56.2	37610			108.431	198530
62.75	47889			114.462	232088
71	63995			120.538	270111
78.75	82473				
83.85	97378				

complete set of data see ref.

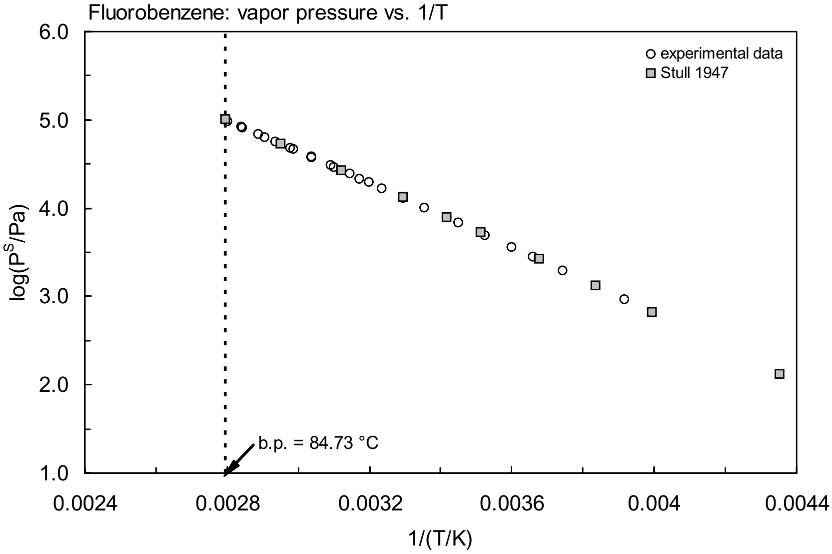
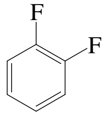


FIGURE 6.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for fluorobenzene.

6.1.3.2 1,2-Difluorobenzene



Common Name: 1,2-Difluorobenzene
Synonym: *o*-difluorobenzene
Chemical Name: 1,2-Difluorobenzene
CAS Registry No: 367-11-3
Molecular Formula: $C_6H_4F_2$
Molecular Weight: 114.093
Melting Point (°C):

–47.1	(Lide 2003)

Boiling Point (°C):

94	(Lide 2003)

Density (g/cm^3 at 20°C):

1.158	(Dean 1992)

Molar Volume (cm^3/mol):

99.2	(calculated-density, Stephenson & Malanowski 1987)
106.0	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

1141	(shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980; Yalkowsky et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9582* (31.17°C, comparative ebulliometry, measured range 31–130°C, Scott et al. 1963)

$\log (P/kPa) = 6.12360 - 1297.243/(211.103 + t/°C)$; temp range 31.2–130°C (Antoine eq. derived from experimental data of Scott et al.1963, Boublik et al. 1984)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

713	(computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.59	(calculated-fragment const., Valvani & Yalkowsky 1980)
2.58	(calculated-fragment const., Yalkowsky et al. 1983)
2.56	(calculated-molar volume correlation, Wang et al. 1992)
2.43	(calculated, Müller & Klein 1992)
2.37	(recommended, Hansch et al. 1995)
2.25; 2.33	(predicted; calc-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:
Half-Lives in the Environment:

TABLE 6.1.3.2.1
Reported vapor pressures of 1,2-difluorobenzene at various temperatures

Scott et al. 1963					
comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa		
31.168	9582	111.903	169053		
33.916	10884	117.980	198530	data also fitted to Cox eq.	
36.668	12335	124.099	232088	Cox eq.	P/mmHg
39.436	13950	130.256	270111	$\log (P/760)=A[1 - B/(T/K)]$	
42.210	15740			$\log A = a - b(T/K) + c(T/K)^2$	
44.996	17725	mp/K	226.0148	a	0.841936
47.803	19920	bp/K	367.07	$10^{-4} \cdot b$	6.77698
53.423	25007	ΔH_{fus} = 11.045 kJ/mol		$10^{-7} \cdot c$	6.52099
59.084	31160	ΔH_V = 36.11 kJ/mol		B	367.072
64.787	38547	Antoine eq.			
70.530	47359	$\log P = A - B/(C + t/°C)$			
76.314	57803		P/mmHg		
82.142	70109	A	7.00003		
88.009	84525	B	1298.053		
93.921	101325	C	221.197		
99.874	120798				
105.869	143268				

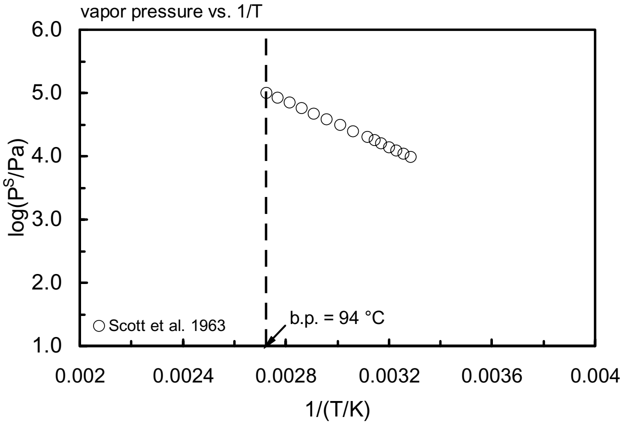
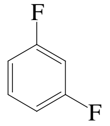


FIGURE 6.1.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2-difluorobenzene.

6.1.3.3 1,3-Difluorobenzene



Common Name: 1,3-Difluorobenzene
Synonym: *m*-difluorobenzene
Chemical Name: 1,3-Difluorobenzene
CAS Registry No: 372-18-9
Molecular Formula: $C_6H_4F_2$
Molecular Weight: 114.093
Melting Point (°C):
–69.12 (Lide 2003)
Boiling Point (°C):
82.6 (Lide 2003)
Density (g/cm^3 at 20°C):
1.1552 (18°C, Horvath 1982)
1.1572 (Lide 2003)
Molar Volume (cm^3/mol):
98.6 (20°C, calculated-density, Stephenson & Malanowski 1987, Ruelle & Kesselring 1997)
106.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
1141 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
19924* (38.284°C, comparative ebulliometry, measured range 311.334–391.523 K, Osborn & Scott 1980)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
2.58 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)
2.56 (calculated-molar volume correlation, Wang et al. 1992)
2.43 (calculated, Müller & Klein 1992)
2.26; 2.33 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:

TABLE 6.1.3.3.1
Reported vapor pressures of 1,3-difluorobenzene at various temperatures

Osborn & Scott 1980			
ebulliometry			
t/°C	P/Pa	t/°C	P/Pa
38.184	19924	88.808	120800
43.646	25014	94.641	143270
49.148	31167	100.511	169050
54.692	38553	106.425	198540
60.273	47363	112.378	232090
65.898	57806	118.373	270120
71.564	70112		
77.272	84528	data fitted to a 4-constant	
83.02	101325	vapor pressure eq.	

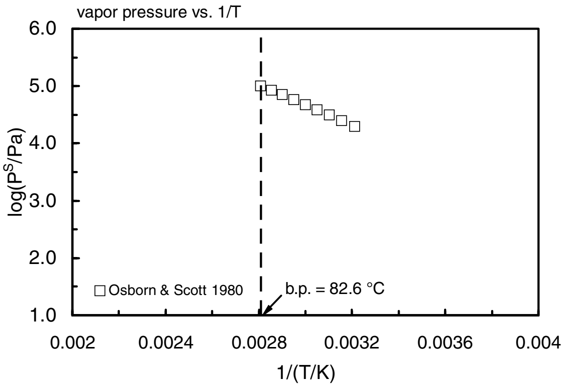
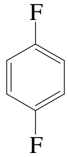


FIGURE 6.1.3.3.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3-difluorobenzene.

6.1.3.4 1,4-Difluorobenzene



Common Name: 1,4-Difluorobenzene
Synonym: *p*-difluorobenzene
Chemical Name: 1,4-Difluorobenzene
CAS Registry No: 540-36-3
Molecular Formula: $C_6H_4F_2$
Molecular Weight: 114.093
Melting Point (°C):

–23.55	(Lide 2003)

Boiling Point (°C):

89	(Lide 2003)

Density (g/cm^3 at 20°C):

1.1701	(20°C, Horvath 1982, Dean 1992; Lide 2003)

Molar Volume (cm^3/mol):

97.4	(20°C, calculated-density, Stephenson & Malanowski 1987)
106.0	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

1222	(shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980; Yalkowsky et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9577*	(27.25°C, comparative ebulliometry, measured temp range 300.4–397.7 K, Osborn & Scott 1980)

Henry's Law Constant (Pa m^3/mol at 25°C):

776	(computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.58	(calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)
2.43	(calculated, Müller & Klein 1992)
2.84	(calculated-molar volume, Wang et al. 1992)
2.24; 2.33	(predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:

TABLE 6.1.3.4.1
Reported vapor pressures of 1,4-difluorobenzene at various temperatures

Osborn & Scott 1980

ebulliometry

t/°C	P/Pa	t/°C	P/Pa
28.248	9577	84.078	84528
30.95	10879	89.886	101325
33.658	12331	95.727	120800
36.376	13944	101.611	143270
39.101	15736	107.535	169050
41.837	17721	113.503	198540
44.588	19924	119.507	232090
50.109	25104	125.552	270120
55.671	31167		
61.273	38553	data fitted to a 4-constant	
66.910	47363	vapor pressure eq.	
72.593	57806		
78.319	70112		

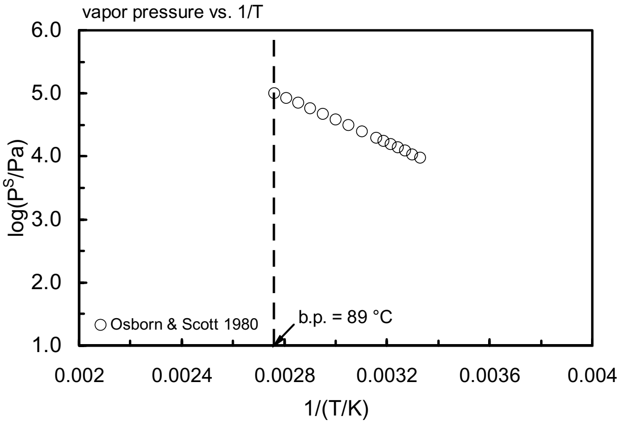
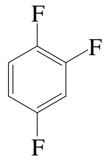


FIGURE 6.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for 1,4-difluorobenzene.

6.1.3.5 1,2,4-Trifluorobenzene



Common Name: 1,2,4-Trifluorobenzene
Synonym:
Chemical Name: 1,2,4-trifluorobenzene
CAS Registry No: 367-23-7
Molecular Formula: $C_6H_3F_3$
Molecular Weight: 132.083
Melting Point (°C):
Boiling Point (°C):

90	(Lide 2003)

Density (g/cm^3):
Molar Volume (cm^3/mol):

111.0	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

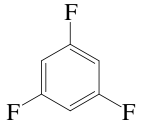
Octanol/Water Partition Coefficient, log K_{OW}:

2.52	(HPLC-RT correlation, Garst 1984, quoted, Sangster 1993)
2.41	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Half-Lives in the Environment:

6.1.3.6 1,3,5-Trifluorobenzene



Common Name: 1,3,5-Trifluorobenzene
Synonym:
Chemical Name: 1,3,5-trifluorobenzene
CAS Registry No: 372-38-3
Molecular Formula: $C_6H_3F_3$
Molecular Weight: 132.083
Melting Point (°C):
–5.5 (Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
75.4 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
103.4 (calculated-density, Stephenson & Malanowski 1987)
111.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
139.68* (25.21°C, static system-Hg manometer, measured range 6.18–50°C, Findlay 1969)
$\log(P/\text{mmHg}) = 6.91873 - 1196.385/(219.01 + t/°C)$; temp range 6.18–50°C (Hg manometer, Findlay 1969)
$\log(P_L/\text{kPa}) = 6.04363 - 1198.385/(-54.131 + T/K)$; temp range 279–350 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:

TABLE 6.1.3.6.1
Reported vapor pressures of 1,3,5-trifluorobenzene at various temperatures

Findlay 1969					
Hg manometer					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
6.18	5385	25.24	13965	46.97	35156
6.19	5389	29.98	17331	46.97	35168
10.03	6615	29.98	17339	49.98	39.453
15.01	8530	35.15	21679	49.99	39.462
15.01	8534	35.25	21806		
19.99	10915	35.39	21846	log P = A – B/(C + t/°C)	
19.99	10911	40.05	26654		P/mmHg
20.49	11.202	40.11	26704	A	6.91873
20.53	11210	43.85	31019	B	1196.385
22.79	12468	43.94	31188	C	219.019
25.21	13968	44.2	31463		

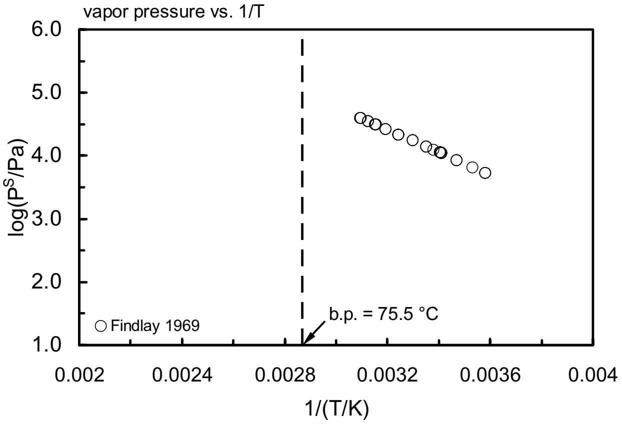
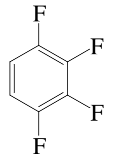


FIGURE 6.1.3.6.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trifluorobenzene.

6.1.3.7 1,2,3,4-Tetrafluorobenzene



Common Name: 1,2,3,4-Tetrafluorobenzene
Synonym:
Chemical Name: 1,2,3,4-tetraflruorbenzene
CAS Registry No: 551-62-2
Molecular Formula: $C_6H_2F_4$
Molecular Weight: 150.074
Melting Point (°C):
–42 (Stephenson & Malanowski 1987)
Boiling Point (°C):
94.3 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
105.5 (calculated-density, Stephenson & Malanowski 1987)
116.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
33.0 (Ambrose et al. 1975)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
6545* (24.82°C, static-system-Hg manometer, Findlay 1969)
log (P/mmHg) = 7.19386 – 1396.067/(228.837 + t/°C); temp range 6.05–49.87°C (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)
6509* (extrapolated from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.15854 – 1291.080/(–50.617 + T/K); temperature range 300.8–367.51(normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.16107 – 1292.550/(–56.453 + T/K); temperature range 300.8–391.65 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.21410 – 1341.655/(223.721 + t/°C); temp range 24.78–84.98°C (Antoine eq. derived from Findlay 1969 data, Boublik et al. 1984)
log (P/kPa) = 6.15932 – 1291.522/(216.58 + t/°C); temp range 27.65–118.5°C (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)
log (P_L/kPa) = 6.31876 – 1396.067/(–44.277 + T/K); temp range 279–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.16042 – 1292.174/(–56.495 + T/K); temp range 300–392 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Half-Lives in the Environment:

TABLE 6.1.3.7.1
Reported vapor pressures of 1,2,3,4-tetrafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Findlay 1969				Ambrose et al. 1975			
Hg manometer				ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
6.05	2385	44.01	15919	27.65	7437	90.123	88.788
6.06	2377	46.91	18024	31.417	8945	94.228	100917
10.36	3041	46.91	18024	35.073	10646	95.082	103593
15.21	3970	48.82	19620	38.868	12.688	99.87	119685
20.64	5277	48.83	19621	42.74	15095	104.196	135850
24.82	6545	49.84	20380	46.466	17757		
24.82	6547	49.87	20.428	51.321	21794	Antoine eq. for temp.	
29.98	8433			55.476	25823	range 300–367 K	
29.99	8433	eq. 2	P/mmHg	60.207	31137	eq. 3	P/kPa
35.05	10722	A	7.19386	64.859	37177	A	6.15854
35.06	10722	B	1396.067	69.749	44535	B	129.08
40.07	13438	C	228.984	75.125	53942	C	–56.617
40.07	13439			79.797	63.331		
43.99	15904			83.34	71.305		

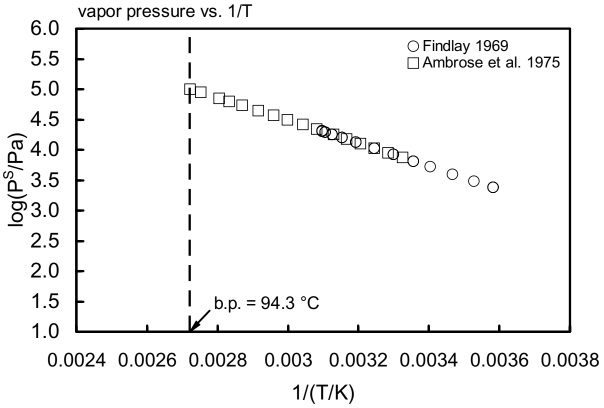
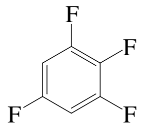


FIGURE 6.1.3.7.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,4-tetrafluorobenzene.

6.1.3.8 1,2,3,5-Tetrafluorobenzene



Common Name: 1,2,3,5-Tetrafluorobenzene
Synonym:
Chemical Name: 1,2,3,5-tetrafluorobenzene
CAS Registry No: 2367-82-0
Molecular Formula: $C_6H_2F_4$
Molecular Weight: 150.074
Melting Point (°C):
–46.25 (Lide 2003)
Boiling Point (°C):
84.4 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
107.7 (20°C, calculated-density, Stephenson & Malanowski 1987)
116.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
32.1 (Ambrose et al. 1975)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
9770* (24.81°C, static method-Hg manometer, measured range 6.08–50°C, Findlay 1969)
log (P/mmHg) = 7.07758 – 1290.984/222.855 + t/°C); temp range 6.08–49.83°C (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)
9801* (interpolated from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.15414 – 1255.781/(–54.898 + T/K); temperature range 287.6–357.61 (normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.15507 – 1255.981/(–54.919 + T/K); temperature range 287.6–381.5 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.12070 – 1250.027/(218.829 + t/°C); temp range 6.08–49.83°C (Antoine eq. derived from Findlay 1969 data, Boublik et al. 1984)
log (P/kPa) = 6.1500 – 1253.079/(217.903 + t/°C); temp range 14.44–108.37°C (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)
log (P_L/kPa) = 6.20248 – 1290.984/(–50.295 + T/K); temp range 279–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.15119 – 1253.771/(–55.168 + T/K); temp range 287–382 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.24644 – 1317.349/(–46.898 + T/K); temp range 385–416 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

TABLE 6.1.3.8.1
Reported vapor pressures of 1,2,3,5-tetrafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C{\cdot}\log (T/K)$	(4)		

Findlay 1969				Ambrose et al. 1975			
Hg manometer				ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
6.05	2385	48.82	19620	287.593	5719	357.291	100305
6.06	2377	48.83	19621	291.414	6987	357.743	101755
10.36	3041	49.84	20380	295.169	8457	362.582	118237
15.21	3970	49.87	20428	298.091	9773	366.716	133926
20.64	5277			303.399	12598	371.603	154528
24.82	6545	eq. 2	P/mmHg	307.963	15541	376.423	177795
24.82	6547	A	7.07758	312.406	18930	381.524	203.907
29.98	8433	B	1290.984	314.635	20846		
29.99	8433	C	223.855	317.751	24802	Antoine eq. for temp range 287–356 K	
35.05	10722			324.852	31779		
35.06	10722			329.202	37666		
40.07	13438			334.506	46007	eq. 2	P/kPa
40.07	13439			338.643	53501	A	6.15414
43.99	15904			343.224	62911	B	1255.781
44.01	15919			347.715	73374	C	–54.898
46.91	18024			352.951	87269		
46.91	18024			356.719	98504		

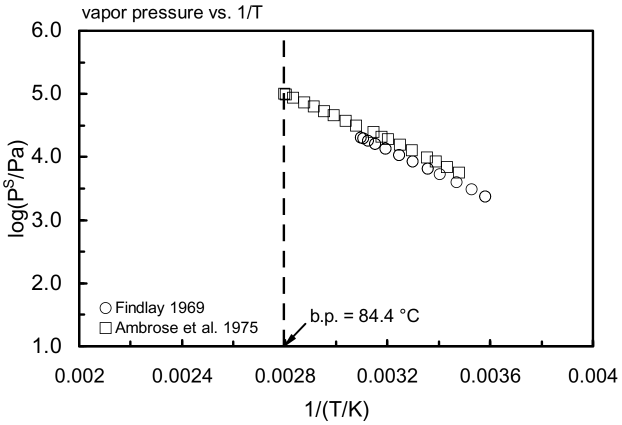
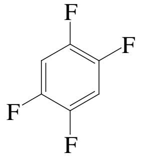


FIGURE 6.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,5-tetrafluorobenzene.

6.1.3.9 1,2,4,5-Tetrafluorobenzene



Common Name: 1,2,4,5-Tetrafluorobenzene
Synonym:
Chemical Name: 1,2,4,5-tetrafluorobenzene
CAS Registry No: 327-54-8
Molecular Formula: $C_6H_2F_4$
Molecular Weight: 150.074
Melting Point (°C):
3.88 (Lide 2003)
Boiling Point (°C):
90.2 (Lide 2003)
Density (g/cm^3 at 20°C):
1.4255 (Lide 2003)
Molar Volume (cm^3/mol):
105.3 (20°C, calculated-density)
105.4 (calculated-density, Stephenson & Malanowski 1987)
116.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
32.9 (Ambrose et al. 1975)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7556* (interpolated from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.17340 – 1277.452/(–56.889 + T/K); temp range 293.2–363.413 (normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.17788 – 1279.904/(–56.642 + T/K); temp range 293.2–387.6 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.17439 – 1277.918/(216.289 + t/°C); temp range 20.05–114.42°C (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)
log (P_L/kPa) = 6.17614 – 1278.93/(–56.748 + T/K); temp range 293–390 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.42009 – 1454.406/(–33.675 + T/K); temp range 390–488 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.88521 – 3090.851/(174.387 + T/K); temp range 488–543 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, $t_{½}$:
Half-Lives in the Environment:

TABLE 6.1.3.9.1
Reported vapor pressures of 1,2,4,5-tetrafluorobenzene at various temperatures:

Ambrose et al. 1975			
ebulliometry			
T/K	**P/Pa**	**T/K**	**P/Pa**
293.198	5855	363.049	100177
296.489	6944	363.591	101.896
300.519	8505	368.237	117566
303.459	9822	372.427	133286
308.374	12399	377.572	154790
313.302	15524	382.398	177330
315.839	17370	387.568	204254
320.056	20841		
324.073	24655	Antoine eq. for temp	
330.275	31652	range 293–363 K	
334.497	37286	log P = A – B/(C + T/K)	
339.931	45699		P/kPa
344.142	53227	A	6.1734
348.439	61895	B	1277.452
353.384	73237	C	–56.889
358.929	87873		
362.593	98750		

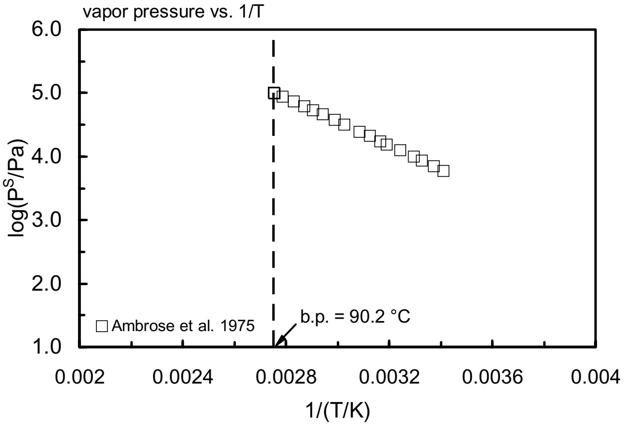
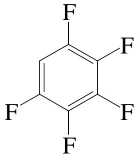


FIGURE 6.1.3.9.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4,5-tetrafluorobenzene.

6.1.3.10 Pentafluorobenzene



Common Name: Pentafluorobenzene
Synonym:
Chemical Name: pentafluorobenzene
CAS Registry No: 363-72-4
Molecular Formula: C_6HF_5
Molecular Weight: 168.064
Melting Point (°C):
–47.4 (Lide 2003)
Boiling Point (°C):
85.74 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
111.0 (20°C, calculated-density, Stephenson & Malanowski 1987)
121.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
32.38 (Ambrose 1968)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
9015* (24.78°C, static method, measured range 24.78–84.98°C, Patrick & Prosser 1964)
log (P/mmHg) = 6.94904 – 1218.91/(213.313 + t/°C); temp range 24.98–84.98°C, Patrick & Prosser 1964)
26584* (48.729°C, ebulliometry, measured range 49–94°C, Ambrose et al. 1975)
log (P/mmHg) = 7.03348 – 1253.043/(215.897 + t/°C); temp range 48.7–94.3°C (Antoine eq. from ebulliometric measurements, Ambrose 1968)
log (P/kPa) = 6.07634 – 1220.72/(213.425 + t/°C); temp range 24.78–84.98°C (Antoine eq. derived from Patrick & Prosser 1946 data, Boublik et al. 1984)
log (P_L/kPa) = 6.15571 – 1250.946/(–57.457 + T/K); temp range 322–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.20712 – 1282.574/(–53.619 + T/K); temp range 358–397 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.47368 – 1477.401/(–27.81 + T/K); temp range 393–479 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
2.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, $t_{½}$:
Half-Lives in the Environment:

TABLE 6.1.3.10.1
Reported vapor pressures of pentafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Patrick & Prosser 1964		Ambrose 1968	
static method-Hg manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
24.78	9015	48.729	26584
29.85	11492	54.355	33360
34.85	14540	59.041	40023
39.85	18206	63.033	46499
44.85	22507	66.698	53178
49.85	27527	69.91	59642
54.87	33877	72.828	66050
59.92	41071	75.604	72643
64.95	49217	78.158	79163
69.95	59052	80.643	85953
74.95	70191	82.998	92792
79.95	82728	85.123	99333
84.98	97125	85.496	100521
		87.212	106123
bp/°C	86.3	89.093	112557
Antoine eq.		91.014	119417
eq. 2	P/mmHg	92.509	124989
A	6.94904	94.296	131878
B	1218.91		
C	213.313	eq. 2	P/mmHg
ΔH_V/(kJ mol^{-1}) =		A	7.03488
at 25°C	36.67	B	1253.043
at bp	32.07	C	215.987

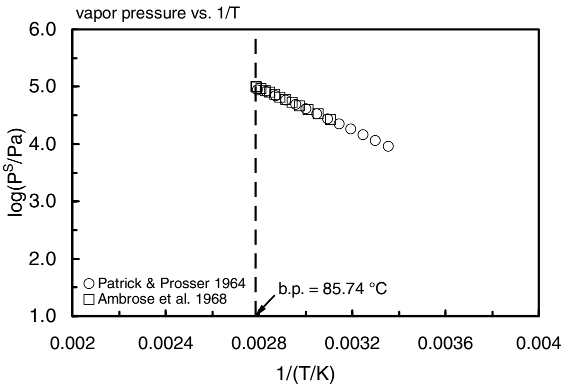
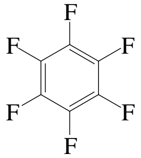


FIGURE 6.1.3.10.1 Logarithm of vapor pressure versus reciprocal temperature for pentafluorobenzene.

6.1.3.11 Hexafluorobenzene



Common Name: Hexafluorobenzene
Synonym: perfluorobenzene
Chemical Name: hexafluorobenzene
CAS Registry No: 392-56-3
Molecular Formula: C_6F_6
Molecular Weight 180.054
Melting Point (°C):
5.0.3 (Lide 2003)
Boiling Point (°C):
80.26 (Lide 2003)
Density (g/cm^3):
1.61866, 1.60732 (20°C, 25°C, Riddick et al. 1986)
1.6184 (20°C, Lide 2003)
Molar Volume (cm^3/mol):
115.8 (calculated-density, Stephenson & Malanowski 1987)
126.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
35.47 (25°C, Findlay 1969)
35.69, 31.67 (25°C, bp, Riddick et al. 1986)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.585 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
11196* (24.78°C, static method, measured range 19.75–84.98°C, Patrick & Prosser 1964)
log (P/mmHg) = 7.39075 – 1432.91/(237.470 + t/°C); temp range 19.76–84.98°C, Patrick & Prosser 1964)
19957* (37.303°C, gas saturation/manometer, measured range 37.303–88.79°C, Counsell et al. 1965)
11402* (25.1°C, Hg manometer, measured range 4.74–47.85°C, Findlay 1969)
log (P/mmHg) = 6.86088 – 1152.442/(208.663 + t/°C); temp range 4.74–47.85 (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)
10733* (24.005°C, ebulliometry, measured range 290–377 K, Ambrose 1981)
log (P/kPa) = 6.05252 – 1177.973/(210.677 + t/°C); temp range 19.75–84.98°C (Antoine eq. derived from Patrick & Prosser 1964 data, Boublik et al. 1984)
log (P/kPa) = 6.14363 – 1220.148/(214.610 + t/°C); temp range 37.3–88.8°C (Antoine eq. derived from Counsell et al. 1965 data, Boublik et al. 1984)
log (P/kPa) = 6.15013 – 1223.989/(215.084 + t/°C); temp range 17–104°C (Antoine eq. derived from Ambrose 1981 data, Boublik et al. 1984)
10733 (selected, Riddick et al. 1986)
log (P/kPa) = 6.14213 – 1219.41/(214.55 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
log (P_S/kPa) = 11.49514 – 3518.13/(44.44 + T/K); temp range 215–278 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.15233 – 1224.974/(–57.984 + T/K); temp range 278–354 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.19544 – 1251.177/(–54.775 + T/K); temp range 348–389 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = –38.8085 – 1.3422 × 10^3/(T/K) + 22.204·log (T/K) – 3.8813 × 10^{-221}·(T/K) + 2.10 × 10^{-5}·$(T/K)^2$; temp range 278–517 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

2.22	(shake flask, Log P Database, Hansch & Leo 1987)
2.22	(recommended, Sangster 1993)
2.54	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constant k = 1.7 × 10^{-5} h^{-1}, 1.32 × 10^{-4} h^{-1}, with H_2O_2 under photolysis at 25°C in F-113 solution and with HO in the gas (Dilling et al. 1988).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{OH} = 2.19 × 10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

k_{OH}(obs) = 2.19 × 10^{-13} cm^3 molecule^{-1} s^{-1}, and k_{OH}(calc) = 1.8 × 10^{-13} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1985)

k_{OH}* = (1.61 ± 0.24) × 10^{-13} cm^3 molecule^{-1} s^{-1} at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

k_{OH}* = 1.72 × 10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

Half-Lives in the Environment:

TABLE 6.1.3.11.1
Reported vapor pressures of hexafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K) (1)
log P = A – B/(C + t/°C) (2)
log P = A – B/(C + T/K) (3)
log P = A – B/(T/K) – C·log (T/K) (4)
ln P = A – B/(T/K) (1a)
ln P = A – B/(C + t/°C) (2a)

Patrick & Prosser 1964		Counsell et al. 1965		Findlay 1969		Ambrose 1981	
static method-Hg manometer		gas saturation/manometer		Hg manometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
19.75	8714	37.303	19957	4.74	3849	290.029	7747
24.78	11196	43.536	26124	5.7	4065	293.503	8940
29.85	14289	49.109	32880	7.07	4426	297.155	10733
34.85	17966	53.82	39638	7.14	4429	300.564	12667
39.85	22461	57.848	46271	9.77	5118	304.801	15466
44.85	27687	61.585	53199	17.23	7646	309.383	19.045

TABLE 6.1.3.11.1 (*Continued*)

Patrick & Prosser 1964		Counsell et al. 1965		Findlay 1969		Ambrose 1981	
static method-Hg manometer		gas saturation/manometer		Hg manometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
49.85	33860	64.655	59496	17.23	7650	313.187	22511
54.87	41446	67.63	66152	19.68	8757	316.417	25904
59.92	50169	70.172	72295	24.28	10915	321.165	31474
64.95	59860	72.666	78764	24.4	10988	325.511	37460
69.95	71569	75.337	86190	25.1	11402	330.676	45736
74.95	84741	77.535	92707	27.08	12511	335.031	53811
80.05	100199	79.632	99284	29.92	14296	339.642	63567
84.98	117109	81.446	105264	29.92	14300	343.774	73469
		83.445	112211	29.92	14303	349.246	88.428
Antoine eq.		85.353	119111	35.92	18822	352.884	88642
eq. 2	P/mmHg	87.027	125463	41.81	24289	353.038	100.13
A	7.39075	88.79	132447	47.32	30456	353.849	102794
B	1432, 91			47.85	31064	358.125	117749
C	237.470	bp/°C	80.261			362.14	133296
		Antoine eq.		eq. 2	P/mmHg	366.773	153.186
bp/°C	80.3	eq. 2	P/mmHg	A	6.86088	371.657	176.601
$\Delta H_V/(\text{kJ mol}^{-1})$ =		A	7.01741	B	1152.442	377.323	207.154
at 25°C	35.75	B	1219.410	C	208.663		
at bp	32.70	C	214.525			eq. 2	P/mmHg
		Kirchhoff eq.				A	
		eq. 4	P/mmHg			B	
		A	22.85552			C	
		B	2524.92				
		C	5.03484				

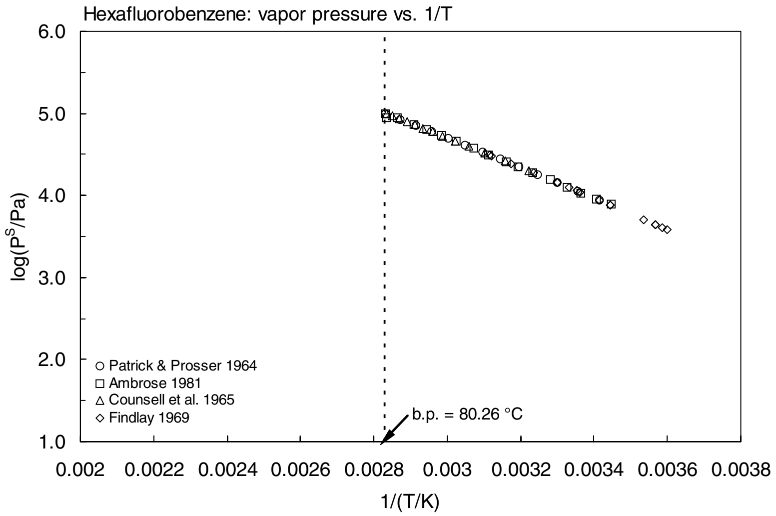
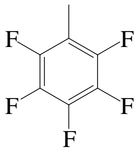


FIGURE 6.1.3.11.1 Logarithm of vapor pressure versus reciprocal temperature for hexafluorobenzene.

6.1.3.12 Pentafluorotoluene



Common Name: Pentafluorotoluene
Synonym: 2, 3, 4, 5, 6-pentafluorotoluene
Chemical Name: 2, 3, 4, 5, 6-pentafluorotoluene
CAS Registry No: 771-56-2
Molecular Formula: $C_7H_3F_5$, $C_6(CH_3)F_5$
Molecular Weight: 182.091
Melting Point (°C):
–29.78 (Lide 2003)
Boiling Point (°C):
117.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.440 (Lide 2003)
Molar Volume (cm^3/mol):
126.5 (20°C, calculated-density, Stephenson & Malanowski 1987)
143.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
35.19 (Ambrose 1968)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
5056* (39.164°C, ebulliometry, measured range 39–138°C or pressure range 30–1500 mmHg, Ambrose 1968)
$\log (P/\text{mmHg}) = 7.07209 - 1384.062/(212.731 + t/°C)$; temp range ~76–127°C or pressure range 200–1000 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)
$\log (P/\text{mmHg}) = 7.09119 - 1388.288/(213.646 + t/°C)$; temp range 39–138°C or pressure range 30–1500 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)
$\log (P/\text{mmHg}) = 13.68523 - 2813.814/(T/K) - 1.2691 \times 10^{-2}\cdot(T/K) + 0.8888\cdot10^{-5}\cdot(T/K)^2$; temp range 39–138°C (Cragoe eq., ebulliometry, Ambrose 1968)
$\log (P_L/\text{kPa}) = 6.19445 - 1382.934/(-60.494 + T/K)$; temp range 312–416 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.21241 - 1394.345/(-59.194 + T/K)$; temp range 348–401 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Half-Lives in the Environment:

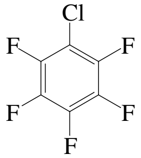
TABLE 6.1.3.12.1
Reported vapor pressures of pentafluorotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\log P = A - B/(T/K) - C \cdot (T/K)^2$ (5)

$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Ambrose 1968			
ebulliometry			
t/°C	P/Pa		
39.164	5056	Antoine eq.	
50.578	8787	eq. 2	P/mmHg
58.357	12354	A	7.09119
62.734	14885	B	1396.198
66.375	17308	C	214.112
72.174	21831	for full range 30–1000 mmHg	
76.551	25854	or temp range 39–138°C	
81.824	31492		
85.651	36176	eq. 2	P/mmHg
92.625	46172	A	7.07209
97.287	54019	B	1384.062
102.370	63757	C	212.731
107.382	66700	for range 200–1000 mmHg	
112.608	87655	or temp range ~76–127°C	
116.158	97433		
117.884	102509	Cragoe eq.	
118.979	105812	eq. 5	P/mmHg
123.337	119831	A	13.68523
127.924	136155	B	2813.814
133.176	156948	C	1.2691×10^{-2}
138.226	179191	D	0.8888×10^{-5}
bp/°C	117.493		
$\Delta H_V = 35.18$ kJ mol^{-1}			

6.1.3.13 Chloropentafluorobenzene



Common Name: Chloropentafluorobenzene
Synonym:
Chemical Name: chloropentafluorobenzene
CAS Registry No: 344-07-0
Molecular Formula: C_6ClF_5
Molecular Weight: 202.509
Melting Point (°C):
Boiling Point (°C):
117.96 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
129.2 (calculated-density, Stephenson & Malanowski 1987)
141.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
35.15 (Ambrose 1968)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
4186* (35.576°C, ebulliometry, measured range 36–144°C or pressure range 30–1500 mmHg, Ambrose 1968)
$\log (P/mmHg) = 7.06976 - 1389.841/(213.833 + t/°C)$; temp range ~80–127°C or pressure range 100–1000 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)
$\log (P/mmHg) = 7.06747 - 1388.288/(213.646 + t/°C)$; temp range 36–144°C or pressure range 30–1500 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)
$\log (P/mmHg) = 14.36999 - 2894.645/(T/K) - 1.4603 \times 10^{-2}\cdot(T/K) + 1.0612\cdot10^{-5}\cdot(T/K)^2$; temp range 36–144°C (Cragoe eq., ebulliometry, Ambrose 1968)
$\log (P_L/kPa) = 6.19201 - 1388.701/(-59.393 + T/K)$: temp range 348–402 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.18873 - 1386.456/(-59.659 + T/K)$, temp range 307–417 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

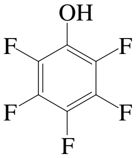
TABLE 6.1.3.13.1
Reported vapor pressures of chloropentafluorotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\log P = A - B/(T/K) - C \cdot (T/K)^2$ (5)

$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Ambrose 1968			
ebulliometry			
t/°C	**P/Pa**		
35.576	4186	Antoine eq.	
44.790	6614	eq. 2	P/mmHg
55.927	11028	A	7.06747
61.852	14216	B	1388.288
65.865	16811	C	213.646
70.085	19929	full range 30–1000 mmHg	
75.343	24459	or temp range 35.6–144°C	
81.691	31024		
86.763	37244	eq. 2	P/mmHg
92.135	44900	A	7.06976
97.254	53331	B	1389.841
102.357	62963	C	213.833
107.155	73251	for range 200–1000 mmHg	
112.764	86927	or temp range ~80–128°C	
116.436	96926		
117.448	99832	Cragoe eq.	
118.893	104118	eq. 5	P/mmHg
125.580	118997	A	14.36999
127.992	134517	B	2894.645
133.467	155905	C	1.4603×10^{-2}
138.689	178705	D	1.0612×10^{-5}
144.131	205189		
bp/°C	117.954		
ΔH_V = 35.15 kJ mol^{-1}			

6.1.3.14 Pentafluorophenol



Common Name: Pentafluorophenol
Synonym:
Chemical Name: pentafluorophenol
CAS Registry No: 771-61-9
Molecular Formula: $C_6(OH)F_5$
Molecular Weight: 184.063
Melting Point (°C):
37.5 (Lide 2003)
Boiling Point (°C):
145.6 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
128.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
41.59 (Ambrose 1968)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.754 (mp at 37.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
26578* (105.448°C, ebulliometry, measured range 105.5–155°C, Ambrose 1968)
log (P/mmHg) = 7.06296 – 1377.185/(183.680 + t/°C); temp range 105–155°C (Antoine eq. from ebulliometric measurements, Ambrose 1968)
log (P_S/kPa) = 11.291 – 3523/(T/K); temp range 273–296 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.18665 – 1377.011/(– 89.435 + T/K); temp range 378–428 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
3.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

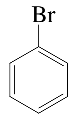
Environmental Fate Rate Constants, k and Half-Lives, $t_{½}$:
Half-Lives in the Environment:

TABLE 6.1.3.14.1
Reported vapor pressures of pentafluorophenol at various temperatures

Ambrose 1968			
ebulliometry			
t/°C	**P/Pa**	**t/°C**	**P/Pa**
105.448	26578	153.041	125269
111.328	32076	154.963	132153
116.192	39393		
120.720	46087	bp/°C	145.621
124.827	52940	ΔH_V = 41.59 kJ mol^{-1}	
128.292	59367	Antoine eq.	
131.565	65904	log P = A − B/(C + t/°C)	
134.647	72670		P/mmHg
137.240	78804	A	7.03488
140.302	86489	B	1253.043
142.507	92412	C	215.897
145.002	99506	full range 200–1000 mmHg	
147.069	105684	or temp range 105–155°C	
149.090	112009		
151.190	118917		

6.1.4 BROMOBENZENES AND BROMOTOLUENES

6.1.4.1 Bromobenzene



Common Name: Bromobenzene
Synonym: phenyl bromide
Chemical Name: bromobenzene
CAS Registry No: 108-86-1
Molecular Formula: C_6H_5Br
Molecular Weight: 157.008
Melting Point (°C):
 –30.72 (Dean 1985; Lide 2003)
Boiling Point (°C):
 156.06 (Dreisbach & Martin 1949; Dreisbach 1955; Lide 2003)
Density (g/cm^3 at 20°C):
 1.4950, 1.48824 (20°C, 25°C, Dreisbach 1955)
 1.4950 (Weast 1982–83; Lide 2003)
 1.4952 (Dean 1985)
Molar Volume (cm^3/mol):
 105.0 (20°C, calculated-density, Chiou 1985)
 119.3 (Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 10.63 (Dreisbach 1955)
 10.70 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 446 (30°C, shake flask-IR, Gross & Saylor 1931)
 410 (shake flask-UV, Andrews & Keefer 1950)
 462 (shake flask-interferometry, Donahue & Bartell 1952)
 328 (Deno & Berkheimer 1960)
 458.5 (35°C, shake flask-UV spectrophotometry, Hine et al. 1963)
 457* (shake flask-spectrophotometry, measured range 10–35°C, Vesala 1973)
 446 (shake flask-UV, Vesala 1974)
 148* (shake flask-GC, measured range 5–45.5°C, Nelson & Smit 1978)
 360 (shake flask-UV, Yalkowsky et al. 1979)
 274* (summary of literature data, temp range 25–40°C, Horvath 1982)
 411 (generator column-HPLC/UV, Wasik et al. 1983)
 330 (headspace-GC, McNally & Grob 1984)
 445* (recommended, temp range 10–40°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)
 $S/(g/kg) = 1.8293 - 1.35675 \times 10^{-2} \cdot (T/K) + 2.99322 \times 10^{-5} \cdot (T/K)^2$; temp range 288–308 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)
 384* (20°C, limiting activity coeff. by equilibrium air stripping-GC, temp range 10–50°C, Hovorka & Dohnal 1997)
 384* (estimated- RP-HPLC-k′ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* (29.8°C, static method-pressure gauge, Kahlbaum 1898)
666.6* (27.8°C, summary of literature data, Stull 1947)
$\log (P/\text{mmHg}) = 7.25422 - 1688.4/(230 + t/°\text{C})$ (Antoine eq., Dreisbach & Martin 1949)
6287* (71.86°C, ebulliometry, measured range 71.86–158.06°C, Dreisbach & Shrader 1949)
3066* (56.07°C, temp range 56.07–154.24°C, Dreyer et al. 1954)
558 (calculated by formula, Dreisbach 1955)
$\log (P/\text{mmHg}) = 6.91444 - 1474.06/(209.4 + t/°\text{C})$; temp range 60–190°C (Antoine eq. for liquid state, Dreisbach 1955)
997 (35°C, gas saturation-gravitational or UV, Hine et al. 1963)
697 (ebulliometry, extrapolated-Antoine eq., measured range 49–131°C, Hammaker & Kerlinger 1969)
$\log (P/\text{mmHg}) = 7.7807 - 2105.4/(T/\text{K})$; temp range 49–131°C (ebulliometry, Hammaker & Kerlinger 1969)
570 (extrapolated-Antoine eq., Weast 1972–73)
$\log (P/\text{mmHg}) = [-0.2185 \times 10157.7/(T/\text{K})] + 8.07500$; temp range –26 to –15°C (Antoine eq., Weast 1972–73)
552 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log (P/\text{mmHg}) = 5.86064 - 1438.817/(205.441 + t/°\text{C})$; temp range 56.07–154°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
553, 555 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 5.99238 - 1443.265/(205.94 + t/°\text{C})$; temp range 56.07–154°C (Antoine eq. from reported exptl. data of Dreyer et al. 1954/55, Boublik et al. 1984)
$\log (P/\text{kPa}) = 5.98225 - 1433.858/(204.562 + t/°\text{C})$; (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
$\log (P/\text{mmHg}) = 6.86064 - 1438.817/(205.441 + t/°\text{C})$; temp range 56–154°C (Antoine eq., Dean 1985, 1992)
557.6 (Riddick e tal. 1986)
$\log (P/\text{kPa}) = 6.37912 - 1688.4/(230 + t/°\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
$\log (P_L/\text{kPa}) = 6.03934 - 1474.03/(-63.75 + T/\text{K})$; temp range 333–463 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.40524 - 1776.58/(-25.639 + T/\text{K})$; temp range 429–633 K (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = -9.4583 - 2.5177 \times 10^3/(T/\text{K}) + 9.2584 \cdot \log (T/\text{K}) - 1.9386 \times 10^{-2} \cdot (T/\text{K}) + 9.6324 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 242–670 K (vapor pressure eq., Yaw et al. 1994)
$\log (P/\text{kPa}) = 5.99238 - 1443.265/(T/\text{K})$ (database of CDATA 1991, Hovorka & Dohnal 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

211 ($1/K_{AW}$ or C_W/C_A, Hine & Mookerjee 1975;)
247 (gas stripping-GC, Mackay & Shiu 1981, 1990)
210 (recommended, Mackay & Shiu 1981)
211 (computer value, Yaws et al. 1991)
256, 332, 579 (30.0, 35, 44.8°C, EPICS-GC, Hansen et al. 1993)
$\ln [H/(\text{kPa}\cdot\text{m}^3/\text{mol})] = -5341/(T/\text{K}) + 16.0$; temp range 30–45°C (EPICS measurements, Hansen et al. 1993)
92.0, 167, 280, 430, 610 (10, 20, 30, 40, 50°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
139 (20°C, selected from literature of experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 6.375 - 2233/(T/\text{K})$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} (at 25°C or as indicated):

2.99 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)
3.03 (calculated-fragment const.; Rekker 1977)
3.16 (HPLC-k′ correlation, McDuffie 1981)
2.98 (generator column-HPLC, Wasik et al. 1983)
3.02 (HPLC-RT correlation, D'Amboise & Hanai 1982)
3.01 (shake flask-GC, Watarai et al. 1982)
3.02 (HPLC-RT correlation, Eadsforth & Moser 1983)

3.01 (HPLC-RT correlation, Garst & Wilson 1984)
3.15 (HPLC correlation, Eadsforth 1986)
2.99 (recommended, Sangster 1989, 1993)
2.75, 2.94 (shake flask-UV/VIS spec. 25, 60°C; Kramer & Henze 1990)
2.99 (recommended, Hansch et al. 1995)
3.29, 3.25, 3.14, 3.12 (5, 15, 25, 35°C, estimated- RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Bioconcentration Factor, log BCF:

3.18 (activated sludge, Freitag et al. 1984)
2.28 (algae, Freitag et al. 1984)
1.68 (fish, Freitag et al. 1984)
1.68, 2.28, 3.18 (fish, algae, activated sludge, Halfon & Reggiani 1986)
1.70 (Freitag et al. 1985)
1.899, 1.928 (calculated-K_{OW}, calculated- MCI χ, Lu et al. 1999)

Sorption Partition Coefficient, log K_{OC}:

2.18 (soil, selected lit., Kenaga & Goring 1980)
2.18 (calculated-S. Kenaga 1980)
2.80 (calculated-MCI χ, Koch 1983)
2.56 (calculated-MCI. Sabjic 1984)
2.65 (calculated-MCI, Bahnick & Doucette 1988)
2.65 (HPLC-RT correlation, cyanopropy column, Hodson & Williams 1988)
3.37 (activated carbon, Blum et al. 1994)
2.49 (soil, calculated-MCI χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}* = 7.3×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at room temp., measured range 245–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

k_{OH}(calc) = 1.3×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs) = 0.71×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH}* = $(9.15 \pm 0.97) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 234–438 K ((flash photolysis-resonance fluorescence, Wallington et al. 1987)

k_{OH} = 7.70×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, independent of temperature over the range 234–362 K (Atkinson 1989)

k_{OH}(calc) = 0.58×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: relative rate from activated sludge approximately of 34.8% CO_2 (Freitag et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 6.1.4.1.1
Reported aqueous solubilities of bromobenzene at various temperatures

$$S(\text{wt\%}) = 1.09002 \times 10^{-2} + 4.43314 \times 10^{-4}\cdot(t/°C) + 1.20007 \times 10^{-5}\cdot(t/°C)^2 - 1.33342 \times 10^{-7}\cdot(t/°C)^3 \quad (1)$$

$$S/(g/kg) = 1.8293 - 1.35675 \times 10^{-2}\cdot(T/K) + 2.99322 \times 10^{-5}\cdot(T/K)^2 \quad (2)$$

1.

Vesala 1973		Nelson & Smit 1978		Horvath 1982		Horvath & Getzen 1985	
shake flask-UV		shake flask-GC		summary of literature data		IUPAC recommended	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
10	389.57	5	1168	25	274	10	387
15.2	406.05	25	148	30	314	15	405
19.6	411.07	39	244	40	393	20	424
25.0	457.19	45.5	314			25	445
30.0	464.56			eq. 1	S/wt%	30	467
35.0	489.19					35	491
						40	516
						eq. 2	S/(g/kg)

2.

Hovorka & Dohnal 1997		Finizio & Di Guardo 2001	
γ^∞ by air stripping-GC		RP-HPLC-k′ correlation	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
10	354.6	5	278
20	384.3	15	274.5
30	427.6	25	384
40	499.0	35	368
50	598.7		

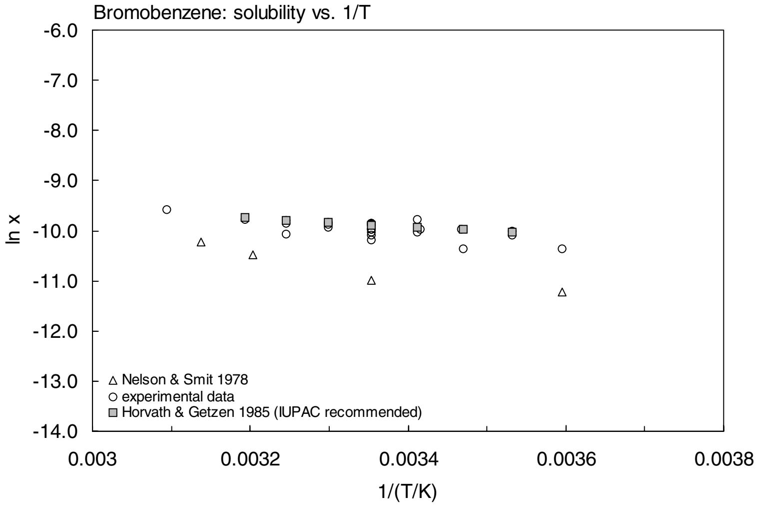


FIGURE 6.1.4.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for bromobenzene.

TABLE 6.1.4.1.2
Reported vapor pressures of bromobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C{\cdot}\log (T/K)$	(4)		

Kahlbaum 1898		**Stull 1947**		**Dreisbach & Shrader 1949**		**Dreyer et al. 1954**	
static method*		**summary of lit. data**		**ebulliometry**			
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
29.8	666.6	2.9	133.3	71.86	6287	56.07	3066
40.6	1333.2	27.8	666.6	76.39	7605	63.52	4400
47.7	1999.8	40	1333	80.08	8851	69.7	5706
52.8	2666.4	53.8	2666	83.99	10114	74.88	7119
57.3	3333	68.6	5333	96.32	16500	78.25	8213
61.2	3999.7	78.1	7999	127.47	42066	81.9	9546
67.7	4666	90.8	13332	140.69	67661	85.55	10986
70.4	5333	110.1	26664	158.06	101325	88.53	12332
73.0	6666.1	132.3	53329			90.82	13426
82.8	9999.2	156.2	101325	bp/°C	156.06	93.49	14839
90.0	13332			mp/°C	–30.82	97.09	16932
109.5	26664	mp/°C	–30.7			99.41	18465
122.0	39997			eq. 2	P/mmHg	101.26	19705
131.6	53329			A	7.25422	105	22425
139.4	66661			B	1688.4	109.5	26118
145.9	79993			C	230	115.59	31877
152.5	93326					122.79	39970
155.5	101325					129.61	49156
						135.48	58275
						139.94	66128
						144.73	75527
						149.51	85433
						151.95	91046
						154.24	96685
						bp/°C	156.083

*complete list see ref.

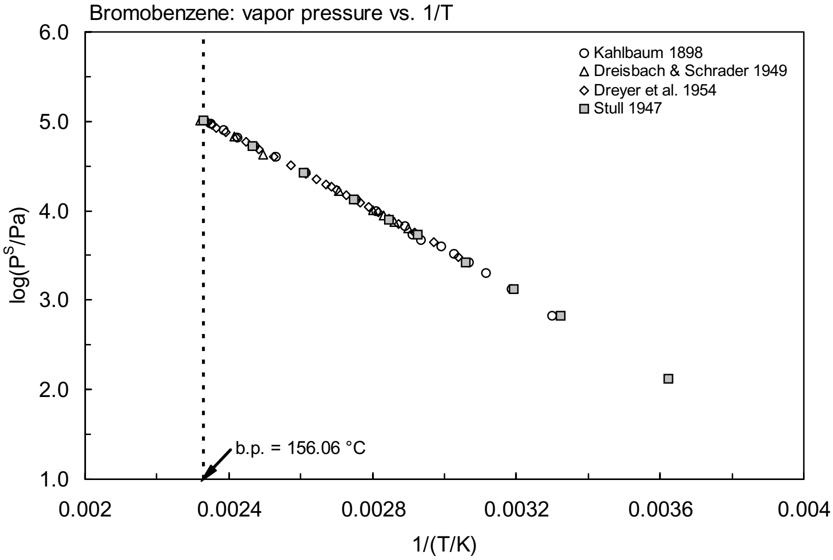
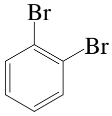


FIGURE 6.1.4.1.2 Logarithm of vapor pressure versus reciprocal temperature for bromobenzene.

6.1.4.2 1,2-Dibromobenzene



Common Name: 1,2-Dibromobenzene
Synonym: *o*-dibromobenzene
Chemical Name: 1,2-Dibromobenzene
CAS Registry No: 583-53-9
Molecular Formula: $C_6H_4Br_2$
Molecular Weight: 235.904
Melting Point (°C):
7.1 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
225 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
1.98429, 1.9767 (20°C, 25°C, Dreisbach 1955)
1.9843 (20°C, Weast 1982–83; Lide 2003)
Molar Volume (cm³/mol):
120.2 (calculated-density, Stephenson & Malanowski 1987)
142.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
59.31, 42.594 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
7.279 (Dreisbach 1955)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
74.55 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
74.8 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
$\log (P/\text{mmHg}) = 7.44451 - 2050.3/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
25.7 (calculated by formula, Dreisbach 1955)
$\log (P/\text{mmHg}) = 7.10265 - 1825.77/(207.0 + t/°C)$; temp range 115–295°C (Antoine eq. for liquid state, Dreisbach 1955)
26.0 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (P/\text{mmHg}) = 7.50128 - 2093.1/(t/°C + 230)$; temp range 28–117°C (Antoine eq., Dean 1985, 1992)
$\log (P/\text{mmHg}) = 7.10265 - 1825.77/(t/°C + 207)$; temp range 117–300°C (Antoine eq., Dean 1985, 1992)
22.80 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
$\log (P/\text{kPa}) = 6.22755 - 1825.77/(T/K - 66.15)$; temp range 388–588 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
3.64 (shake flask, Hansch & Leo 1979; Hansch et al. 1995)
3.68 (HPLC-RT correlation, Garst & Wilson 1984)
3.64 (recommended, Sangster 1993)
3.64 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

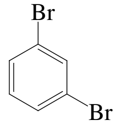
2.70; 3.50 (*Pimephales promelas; Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.4.3 1,3-Dibromobenzene



Common Name: 1,3-Dibromobenzene
Synonym: *m*-dibromobenzene
Chemical Name: 1,3-Dibromobenzene
CAS Registry No: 108-36-1
Molecular Formula: $C_6H_4Br_2$
Molecular Weight: 235.904
Melting Point (°C):
–7.0 (Weast 1982–83; Stephenson & Malanlowski 1987; Lide 2003)
Boiling Point (°C):
218 (Lide 2003)
Density (g/cm^3 at 20°C):
1.9523 (20°C, Weast 1982–83; Lide 2003)
Molar Volume (cm^3/mol):
120.8 (20°C, calculated-density, Stephenson & Malanowski 1987)
142.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
67.4 (30°C, shake flask-UV, Hine et al. 1963)
98.45 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
64.0 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
57.06 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)
22.78 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P/kPa) = 5.971 - 1603.4/(T/K - 87.55)$; temp range 417–500 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
157, 61.05 (calculated-$\Delta S_{v,}$ mp and bp, Antoine eq., Yalkowsky & Mishra 1990, Mishra & Yalkowsky 1991)
$\log (P/mmHg) = 59.2974 - 4.6960 \times 10^3/(T/K) - 18.444\cdot\log (T/K) + 6.7598 \times 10^{-3}\cdot(T/K) - 2.5567 \times 10^{-13}\cdot(T/K)^2$; temp range 226–761 K (vapor pressure eq., Yaw et al. 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
3.75 (shake flask, Hansch & Leo 1979; Hansch et al. 1995)
3.79 (shake flask-GC, Watarai et al. 1982)
3.78 (Oliver & Niimi 1984)
3.74 (HPLC-k′ correlation, Haky & Yeung 1984)
3.75 (recommended, Sangster 1993)
3.75 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
2.78 (mean value, rainbow trout, Oliver & Niimi 1984)
2.82 (rainbow trout, Oliver 1987)
2.82 (*Oncorhynchus mykiss*, under flow-through conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: pseudo-first order reaction rate constant for direct photolysis k = 0.009 min^{-1} with $t_{½}$ = 76.8 min. in dilute aqueous solution (Peijnenburg et al. 1992).

Half-Lives in the Environment:

Air:

Surface water: pseudo-first order reaction rate constant for direct photolysis k = 0.009 min^{-1} with $t_{½}$ = 76.8 min. in dilute aqueous solution (Peijnenburg et al. 1992).

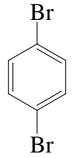
Groundwater:

Sediment:

Soil:

Biota: $t_{½}$ = 3 d (guppy, Niimi 1987)

6.1.4.4 1,4-Dibromobenzene



Common Name: 1,4-Dibromobenzene
Synonym: *p*-dibromobenzene
Chemical Name: 1,4-Dibromobenzene
CAS Registry No: 106-37-6
Molecular Formula: $C_6H_4Br_2$
Molecular Weight: 235.904
Melting Point (°C):
  87.43 (Lide 2003)
Boiling Point (°C):
  218.5 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.5742 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
  121 (calculated-density, Lande & Banerjee 1981)
  142.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  4.837 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.244 (mp at 87.43°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
  20.0 (shake flask-UV, Andrews & Keefer 1950)
  26.42 (35°C, shake flask-UV spectrophotometry, Hine et al. 1963)
  20.08 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
  20.0 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)
  17.0* (shake flask-HPLC, measured range 10–35°C, Kuramochi et al. 2004)
  ln [S/(mol/L)] = –3151.3.7/(T/K) + 1.06; temp range 10–35°C (shake flask-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  133.3* (61°C, summary of literature data, Stull 1947)
  log (P/mmHg) = 7.44830 – 2057.2/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
  9.33* (25.8°C, manometer, temp range 25.8–80.5°C, Walsh & Smith 1961)
  log (P/mmHg) = 11.592 –3826.2/(T/K); temp range 25.8–80.5°C (manometer, Walsh & Smith 1961)
  17.87 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)
  log (P/mmHg) = [–0.2185 × 13047.8/(T/K)] + 8.769771; temp range 61–218.6°C (Antoine eq., Weast 1972–73)
  3.96* (18.13°C, capacitance manometer; De Kruif et al. 1981)
  7.65 (interpolated, Antoine eq., Stephenson & Malanowski 1987)
  log P/kPa = 10.717 – 3826.2/(T/K); temp range 298–354 K (Antoine eq., solid, Stephension & Malanowski 1987)
  log P/kPa = 6.5732 – 2047.2/(T/K – 43.15); temp range 373–493 K (Antoine eq., liquid, Stephenson & Malanwoski 1987)
  35.95, 53.18 (calculated-bp, Antoine eq., Yalkowsky & Mishra 1990)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  106 (derived from γ_W, infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:

3.75	(shake flask, Hansch & Leo 1979)
4.07	(calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980)
4.13	(calculated-fragment const., Yalkowsky et al. 1983)
3.79	(shake flask-GC, Watarai et al. 1982)
3.89	(Gobas et al. 1989)
3.79	(recommended, Sangster 1993)
3.79	(recommended, Hansch et al. 1995)
3.62	(GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

5.21	(calculated-S_{oct} and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

3.15	(guppy, lipid-weight based, Gobas et al. 1989)
1.96	(*Poecilia reticulata*, under flow-through conditions, Devillers et al. 1996)
2.70; 3.40	(*Poecilia reticulata; Pimephales promelas*, under static and semi-static conditions, Devillers et al. 1996)
3.15	(Gobas et al. 1989)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
log k_1 = 2.11 d^{-1}; log k_2 = 0.15 d^{-1} (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

TABLE 6.1.4.4.1
Reported aqueous solubilities and vapor pressures of 1,4-dibromobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log (P/mmHg) = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log (P/Pa) = A - B/(C + T/K)$	(3)		
$\log (P/mmHg) = A - B/(T/K) - C\cdot\log (T/K)$	(4)		

Aqueous solubility		Vapor pressure					
Kuramochi et al.2004		Stull 1947		Walsh & Smith 1961		de Kruif et al. 1981	
shake flask-GC		summary of literature data		manometry		diaphragm gauge	
t/°C	S/(g m^{-3})	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
10	9.91	61.0	133.3	25.8	9.33	1.54	0.617
25	17.0	79.3	666.6	26.8	9.33	3.93	0.829
35	24.6	87.7	1333	27.5	10.67	3.95	0.832
		103.6	2666	31.9	14.67	7.62	1.253
mp/°C	84.55	120.8	5333	38.1	26.66	10.54	1.736
		131.6	7999	42.6	38.66	14.02	2.544
$\Delta H_{sol}/(kJ\ mol^{-1}) = 26.2$		146.5	13332	42.6	40.0	18.13	3.960
$\Delta H_{fusl}/(kJ\ mol^{-1}) = 18.6$		168.5	26664	44.6	48.0		
		192.5	53329	50.2	73.33		
		218.6	101325	51.2	83.99	eq. 1	P/Pa

(*Continued*)

TABLE 6.1.4.4.1 (*Continued*)

Aqueous solubility		Vapor pressure					
Kuramochi et al.2004		Stull 1947		Walsh & Smith 1961		de Kruif et al. 1981	
shake flask-GC		summary of literature data		manometry		diaphragm gauge	
t/°C	S/(g m^{-3})	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
ln S = –3151.3/(T/K) + 1.06				56.4	129.3	A	13.86395
S in mol/L		mp/°C	87.5	57.2	136.0	B	3864.8
				57.3	141.3		
				64.3	238.7		
				71.8	420.0		
				80.5	791.9		
				mp/°C	87.24		
				eq. 1	P/mmHg		
				A	11.592		
				B	3826.2		
				ΔH_{subl}/(kJ mol^{-1}) = 73.26			

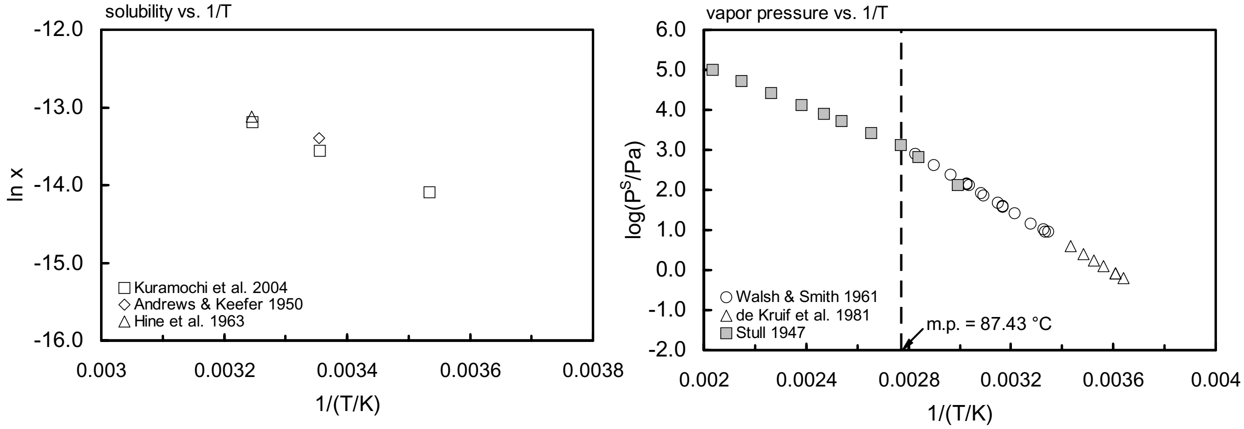
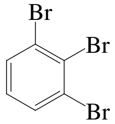


FIGURE 6.1.4.4.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,4-dibromobenzene.

6.1.4.5 1,2,3-Tribromobenzene



Common Name: 1,2,3-Tribromobenzene
Synonym:
Chemical Name: 1,2,3-tribromobenzene
CAS Registry No: 608-21-9
Molecular Formula: $C_6H_3Br_3$
Molecular Weight: 314.800
Melting Point (°C):
  87.8 (Weast 1982–83)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
  2.658 (Weast 1982–83, Horvath 1982)
Molar Volume (cm^3/mol):
  137.7 (Ruelle & Kesselring 1997)
  118 (calculated-density, Wang et al. 1992)
  165.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.242 (mp at 87.8°C)

Water Solubility (g/m^3 or mg/L at 25°C):
  2.94 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
  4.98; 4.25 (quoted exptl value; calculated-molar volume, Wang et al. 1992)
  4.57; 4.42 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

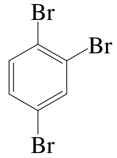
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
  Biota: $t_{1/2}$ = 3 d in guppy (for tribromobenzenes, Niimi 1986).

6.1.4.6 1,2,4-Tribromobenzene



Common Name: 1,2,4-Tribromobenzene
Synonym:
Chemical Name: 1,2,4-tribromobenzene
CAS Registry No: 615-54-3
Molecular Formula: $C_6H_3Br_3$
Molecular Weight: 314.800
Melting Point (°C):
  44.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
  275 (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  137.7 (Ruelle & Kesselring 1997)
  165.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.644 (mp at 44.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  9.96 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
  10.1 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)
  3.67, 7.21, 11.0 (10, 25, 35°C, generator column-HPLC, Kuramochi et al. 2004)
  $\ln [S/(mol/L)] = -3836.9/(T/K) + 2.19$; temp range 10–35°C (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):
  31.9 (derived from γ_W, infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
  4.51 (shake flask-GC, Watarai et al. 1982)
  4.54 (Oliver & Niimi 1984)
  4.32 (GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:

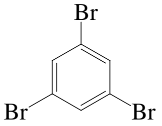
Bioconcentration Factor, log BCF:
  3.63 (rainbow trout, Oliver 1984, Oliver & Niimi 1984, Oliver 1987)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
  Biota: $t_{1/2}$ = 3 d in guppy (for tribromobenzenes, Niimi 1987)

6.1.4.7 1,3,5-Tribromobenzene



Common Name: 1,3,5-Tribromobenzene
Synonym:
Chemical Name: 1,3,5-tribromobenzene
CAS Registry No: 626-39-1
Molecular Formula: $C_6H_3Br_3$
Molecular Weight: 314.800
Melting Point (°C):

122.8	(Lide 2003)

Boiling Point (°C):

271	(Weast 1982–83; Lide 2003)

Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

137.7	(Ruelle & Kesselring 1997)
165.9	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.11 (mp at 122.8°C)

Water Solubility (g/m^3 or mg/L at 25°C):

200	(shake flask-residue volume method, Booth & Everson 1948)
0.04	(Stephen & Stephen 1963)
0.787	(shake flask-UV, Yalkowsky et al. 1979)
0.789	(recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)

Vapor Pressure (Pa at 25°C):

5.187	(GC-RT correlation, Watanabe & Tatsukawa 1989)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

4.51	(shake flask-GC, Watarai et al. 1982)
5.07	(calculated-fragment const., Yalkowsky et al. 1983)
4.60, 4.63	(HPLC-RT correlation, Garst 1984)
5.26	(HPLC-RT correlation, Gobas et al. 1989)
5.18	(reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
4.51	(recommended, Sangster 1993)
4.51	(selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

3.70 (rainbow trout, Oliver & Niimi 1984, Oliver 1987)
3.26–4.08 mean 3.97; 3.53–4.20 mean 4.08 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)
4.42 (guppy, lipid-weight based, Gobas et al. 1989)
3.23; 3.70, 3.97, 4.08 (*Poecilia reticulata; Oncorhynchus mykiss,* quoted values, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: pseudo-first order reaction rate constant in dilute aqueous solution $k = 0.005\ min^{-1}$ with $t_{½} = 140.5$ min. (Peijeneburg et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$\log k_1 = 2.85\ d^{-1}$; $\log k_2 = -0.38\ d^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Air:

Surface water: pseudo-first order reaction rate constant for direct photolysis in dilute aqueous solution $k = 0.005\ min^{-1}$ with $t_{½} = 140.5$ min. (Peijeneburg et al. 1992).

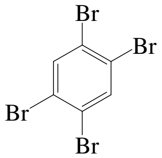
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{½} = 3$ d (guppy, for tribromobenzenes, Niimi 1987)

6.1.4.8 1,2,4,5-Tetrabromobenzene



Common Name: 1,2,4,5-Tetrabromobenzene
Synonym:
Chemical Name: 1,2,4,5-tetrabromobenzene
CAS Registry No: 636-28-2
Molecular Formula: $C_6H_2Br_4$
Molecular Weight: 393.696
Melting Point (°C):
  182 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
  3.072 (Weast 1982–83)
Molar Volume (cm^3/mol):
  128.2 (calculated-density, Wang et al. 1992)
  153.8 (Ruelle & Kesselring 1997)
  189.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0288 (mp at 182°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  0.0433 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
  0.0434 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)
  0.044 (shake flask-GC, Kim & Saleh 1990)
  0.0182, 0.0435, 0.0778 (10, 25, 35°C, generator column-HPLC, Kuramochi et al. 2004)
  $\ln [S/(mol/L)] = -4967.5/(T/K) + 0.681$; temp range 10–35°C (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at 25°C):
  0.157 (GC-RT correlation, Watanabe & Tatsukawa 1989)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  376 (derived from γ_W, infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
  5.13 (shake flask-GC, Watarai et al. 1982)
  5.25 (HPLC-RT correlation, Garst 1984)
  5.56 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  5.13 (recommended, Sangster 1993)
  5.13 (recommended, Hansch et al. 1995)
  5.00 (GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
  3.80 (rainbow trout, Banerjee et al. 1980)
  2.94–3.68 mean 3.57; 3.40–3.91 mean 3.81 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)

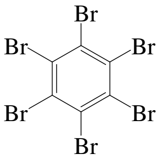
3.80 (Nendza 1993; quoted, Lu et al. 1999)
3.57 (*Oncorhynchus mykiss*, flow through conditions, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
Biota: $t_{1/2}$ = 4 d in guppy (for tetrabromobenzenes, Niimi 1987)

6.1.4.9 Hexabromobenzene



Common Name: Hexabromobenzene
Synonym:
Chemical Name: hexabromobenzene
CAS Registry No: 87-82-1
Molecular Formula: C_6Br_6
Molecular Weight: 551.488
Melting Point (°C):
  327 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  186 (Ruelle & Kesselring 1997)
  235.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  85 (Tittlemier et al. 2002)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0011 (mp at 327°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and the reported temperature dependence equations):
  0.00016 (22°C, generator column-GC, Opperhuizen 1986)
  0.0030 (generator column-GC/ECD, Tittlemier et al. 2002)
  0.0000472, 0.00011, 0.000232 (10, 25, 35°C, generator column-HPLC, Kuramochi et al. 2004)
  $\ln [S/(mol/L)] = -5484.7/(T/K) - 3.85$; temp range 10–35°C (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
  3.133×10^{-4} (estimated, Lyman et al. 1982)
  3.845×10^{-4} (GC-RT correlation, Watanabe & Tatsukawa 1989)
  7.50×10^{-4} (supercooled liquid P_L, GC-RT correlation, Tittlemier et al. 2002)
  $\log (P_L/Pa) = -4454/(T/K) + 11.82$ (Clauius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):
  0.284 (calculated, Meylan & Howard 1991)
  0.14 (calculated-P_L/C_L, Tittlemier et al. 2002)
  10.8 (derived from γ_W, infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
  6.15, 6.07 (HPLC-RT correlation, Garst 1984)
  7.80 (HPLC-RT correlation, Opperhuizen 1986)
  > 6.0 (estimated, Gobas et al. 1987)
  7.06 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  6.07 (recommended, Sangster 1993)
  6.07 (Hansch et al. 1995)
  6.07 (GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.95–3.08 mean 3.04 (rainbow trout, wet wt., 15°C, steady-state BCF on 21- to 96-d laboratory study, Oliver & Niimi 1985)

1.0	(Kawasaki 1980)
5.0	(Nendza 1993)
4.892, 4.681	(calculated-MCI, calculated-K_{OW}, Lu et al. 1999)

Sorption Partition Coefficient, log K_{OC}:

4.45, 4.68 (estimated-solubility, Lyman et al. 1982; quoted, K_{OW}, Howard 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated volatilization $t_{1/2}$ = 3.3 d from a model river is 3.3 d, $t_{1/2}$ = 114 months from a model pond with adsorptive processes (Howard 1997)

Photolysis: not expected to occur (Howard 1997)

Oxidation: not expected to occur (Howard 1997)

Hydrolysis: not expected to occur (Howard 1997)

Half-Lives in the Environment:

Air:

Surface water: estimated volatilization $t_{1/2}$ = 3.3 d from a model river, $t_{1/2}$ = 114 months from a model pond with adsorptive processes (Howard 1997)

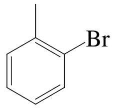
Groundwater:

Sediment:

Soil:

Biota:

6.1.4.10 2-Bromotoluene



Common Name: 2-Bromotoluene
Synonym: *o*-bromotoluene, 1-bromo-2-methylbenzene
Chemical Name: 2-bromotoluene
CAS Registry No: 95-46-5
Molecular Formula: C_7H_7Br
Molecular Weight: 171.035
Melting Point (°C):
– 27.8 (Weast 1982–82; Lide 2003)
Boiling Point (°C):
181.7 (Dreisbach 1959; Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.42322, 1.41774 (20°C, 25°C, Dreisbach 1959)
1.4232 (Weast 1982–83; Lide 2003)
Molar Volume (cm^3/mol):
120.2 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
141.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
49.264, 38.995 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
2.423 (Dreisbach 1955)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
51.3 (estimated, Howard 1997)
1007; 105 (quoted, calculated-molar volume and mp, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
186 (interpolated-Antoine eq., Stuckey & Saylor 1940)
log P/mmHg = 7.50879 – 1913.46/(T/K – 38.34); temp range 4–75°C (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)
133.3* (24.4, summary of lit. data, Stull 1947)
181 (calculated by formula., Dreisbach 1955)
log (P/mmHg) = 6.90847 – 1549.39/(C + t/°C); temp range 80–245°C, (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = [–0.2185 × 11365.0/(T/K)] + 8.396578; temp range 24.4–181.8°C (Antoine eq., Weast 1972–73)
log (P_L/kPa) = 6.03337 – 1549.39/(T/K – 70.15); temp range 353–518 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
242 (estimated-group contribution method, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
2.92 (Hansch & Leo 1979, Hansch et al. 1995)
3.61 (HPLC-k′ correlation, Hanai et al. 1981)
3.43 (estimated, Howard 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

2.38 (estimated-K_{OW}, Howard 1997)

Sorption Partition Coefficient, log K_{OC}:

2.96 (estimated, Howard 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 1.7 h from a model river 1-m deep and $t_{1/2}$ = 14.9 d from a pond (Howard 1997).
Photolysis:
Oxidation: atmospheric $t_{1/2}$ ~ 6.2 d for reaction with hydroxyl radicals in air (Howard 1997).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

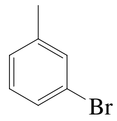
Half-Lives in the Environment:

Air: atmospheric $t_{1/2}$ ~ 6.2 d for reaction with OH radicals in air (Howard 1997).
Surface water: volatilization $t_{1/2}$ = 1.7 h from a model river 1-m deep flowing 1 m/s with a wind speed of 5 m/s and $t_{1/2}$ = 14.9 d from a model pond with adsorption from water column (Howard 1997).

TABLE 6.1.4.10.1
Reported vapor pressures of 2-bromotoluene at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
24.4	133.3
49.7	666.6
62.3	1333
76.0	2666
91.0	5333
100.0	7999
112.0	13332
133.6	26664
157.3	53329
181.8	101325
mp/°C	–28

6.1.4.11 3-Bromotoluene



Common Name: 3-Bromotoluene
Synonym: *m*-bromotoluene
Chemical Name: 3-bromotoluene
CAS Registry No: 591-17-3
Molecular Formula: C_7H_7Br
Molecular Weight: 171.035
Melting Point (°C):
  –39.8 (Lide 2003)
Boiling Point (°C):
  183.7 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.4099 (Lide 2003)
Molar Volume (cm^3/mol):
  121.3 (20°C, calculated-density, Stephenson & Malanowski 1987)
  141.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  51.3 (estimated, Howard 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  133.3* (14.8°C, summary of lit. data, Stull 1947)
  $\log P/\text{mmHg} = 7.75409 - 2049.14/(T/K - 31.44)$; temp range 4–75°C (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)
  $\log (P/\text{mmHg}) = [-0.2185 \times 10537.1/(T/K)] + 7.886560$; temp range 14.8–183.7°C (Antoine eq., Weast 1972–73)
  145 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_L/\text{kPa}) = 6.86228 - 2085.49/(T/K - 27.333)$; temp range: 287–457 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  445 (estimated-P/C, Howard 1997)

Octanol/Water Partition Coefficient, log K_{OW}:
  3.43 (estimated, Howard 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
  2.38 (estimated-K_{OW}, Howard 1997)

Sorption Partition Coefficient, log K_{OC}:
  2.96 (estimated, Howard 1997)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 1.5 h and 14.9 d from a model river 1-m deep and $t_{½}$ = 14.9 d from a pond (Howard 1997).
Photolysis:
Oxidation: atmospheric $t_{½}$ ~ 3 d for reaction with hydroxyl radical in air (Howard 1997).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

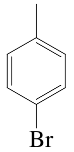
Half-Lives in the Environment:

Air: atmospheric $t_{½}$ ~3 d half-life for reaction with hydroxyl radical in air (Howard 1997).
Surface water: volatilization $t_{½}$ = 1.5 h from a model river 1 m deep flowing 1 m/s with a wind speed of 5 m/s) and $t_{½}$ = 14.9 d in a model pond with adsorption, from water column (Howard 1997).

TABLE 6.1.4.11.1
Reported vapor pressures of 3-bromotoluene at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
14.8	133.3
50.8	666.6
64.0	1333
78.1	2666
93.9	5333
104.1	7999
117.8	13332
138.0	26664
160.0	53329
183.7	101325
mp/°C	–39.8

6.1.4.12 4-Bromotoluene



Common Name: 4-Bromotoluene
Synonym: *p*-bromotoluene, 4-bromo-1-methylbenzene
Chemical Name: *p*-bromotoluene
CAS Registry No: 106-38-7
Molecular Formula: C_7H_7Br
Molecular Weight: 171.042
Melting Point (°C):

28.5	(Lide 2003)

Boiling Point (°C):

184.3	(Lide 2003)

Density (g/cm^3 at 25°C):

1.39953	(Dreisbach 1955)

Molar Volume (cm^3/mol):

122.5	(Ruelle & Kesselring 1997)
141.5	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
49.74, 39.98 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.82	(Dreisbach 1955)
3.5684	(Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

110	(Hine & Mookerjee 1975)
110; 81.9	(quoted; calculated-molar volume and mp, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (10.3°C, summary of lit. data, Stull 1947)
153.2 (calculated by formula., Dreisbach 1955)
$\log (P/mmHg) = 7.00762 - 1612.35/(206.36 + t/°C)$; temp range 85–250°C (Antoine eq. for liquid state, Dreisbach 1955)
$\log (P/mmHg) = 7.00762 - 1612.35/(t/°C + 206.36)$; temp range 85–280°C (Antoine eq., Dean 1985, 1992)
$\log (P/kPa) = 6.13252 - 1612.35/(T/K - 66.79)$; temp range 358–523 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = 12.8209 - 2.6568 \times 10^3/(T/K) - 1.4314\cdot\log (T/K) - 8.9677 \times 10^{-4}\cdot(T/K) + 3.9733 \times 10^{-7}\cdot(T/K)^2$, temp range 300–699 K (Yaws 1994)

Henry's Law Constant ($Pa\cdot m^3/mol$ at 25°C):

23.82	(calculated-P/C, Howard 1997)

Octanol/Water Partition Coefficient, log K_{OW}:

3.42	(quoted, Howard 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

2.54 (calculated-K_{OW}, Howard 1997)

Sorption Partition Coefficient, log K_{OC}:

3.10–3.27 (estimated, Howard 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: $t_{½}$ ~ 9.4 d for reaction with OH radical in the atmosphere (Howard 1997).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

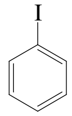
Air: atmospheric $t_{½}$ ~ 9.4 d for reaction with OH radical (Howard 1997).
Surface water: volatilization $t_{½}$ = 4.3 h from a model river 1 m deep and $t_{½}$ = 14.9 d from an environmental pond (Howard 1997).

TABLE 6.1.4.12.1
Reported vapor pressures of 4-bromotoluene at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
10.3	133.3
47.5	666.6
61.1	1333
75.2	2666
91.8	5333
102.3	7999
116.4	13332
137.4	26664
160.2	53329
184.5	101325
mp/°C	28.5

6.1.5 IODOBENZENES

6.1.5.1 Iodobenzene



Common Name: Iodobenzene
Synonym: phenyl iodide
Chemical Name: iodobenzene
CAS Registry No: 591-50-4
Molecular Formula: C_6H_5I
Molecular Weight: 204.008
Melting Point (°C):
–31.3 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
188.4 (Lide 2003)
Density (g/cm^3 at 20°C):
1.8308 (Weast 1982–83; Lide 2003)
1.8308, 1.8229(20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
111.4 (20°C, calculated-density, Stephenson & Malanowski 1987; Wang et al. 1992)
129.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
40.794 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
340 (30°C, Gross et al. 1933)
180 (shake flask-UV spectrophotometry, Andrews & Keefer 1950)
228* (25.1°C, shake flask-spectrophotometry, measured range 10–35°C, Vesala 1973)
229 (shake flask-UV spectrophotometry, Vesala 1974)
158 (Deno & Berkheimer 1960)
95* (shake flask-GC, measured range 5–45.5°C, Nelson & Smit 1978)
267.6* (summary of literature data, temp range 25–50 °C, Horvath 1982)
201 (Miller et al. 1985)
226* (recommended, temp range 10–45°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)
$S/(g/kg) = 0.59293 - 4.8616 \times 10^{-3} \cdot (T/K) + 1.21754 \times 10^{-5} \cdot (T/K)^2$; temp range 283–318 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
213* (29.3°C, Ramsay-Young method, measured range 29.3–100.35°C, Young 1889)
133.3*, 666.6 (24.1, 50.6°C, summary of lit. data, temp range 24.1–188.6°C, Stull 1947)
134.5 (calculated by formula, Dreisbach 1955)
$\log (P/mmHg) = 6.89506 - 1562.87/(201.0 + t/°C)$; temp range: 85–270°C (Antoine eq. for liquid state, Dreisbach 1955)
132.0 (Antoine eq., Boublik et al. 1973)
$\log (P/mmHg) = 7.01187 - 1640.124/(208.765 + t/°C)$; temp range 29.3–188.2°C (Antoine eq. from reported exptl. data of Young 1889, Boublik et al. 1973)
134 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.15935 – 1656.226/(210.496 + t/°C); temp range 29.3–188.2°C (Antoine eq. from reported exptl. data of Young 1889, Boublik et al. 1984)
log (P/mmHg) = 7.0119 – 1640.1/(208.8 + t/°C); temp range 20–188°C (Antoine eq., Dean 1985, 1992)
134.5 (Riddick et al. 1986)
133 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.01996 – 1562.87/(– 72.15 + T/K); temp range 358–543 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.46493 – 1867.69/(–20.202 + T/K); temp range 462–679 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.36129 – 1765.99/(– 54.15 + T/K); temp range 273–358 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = 32.7342 – 3.5824 × 10^3/(T/K) – 8.4197·log (T/K) + 2.0073 × 10^{-10}·(T/K) + 1.591 × 10^{-6}·$(T/K)^2$; temp range 242–721 K (Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

130	(recommended, Mackay & Shiu 1981)
134	(computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

3.25, 3.32	(quoted, calculated-fragment const., Rekker 1977)
3.25	(Hansch & Leo 1979)
3.28	(generator column-HPLC, Wasik et al. 1983)
3.28	(generator column-HPLC, Tewari et al. 1982)
3.23	(HPLC/MS correlation, Burkhard et al. 1985)
3.37	(HPLC-RT correlation, Eadsforth 1986)
3.25	(recommended, Sangster 1989)
3.25	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k_{OH}(calc) = 1.3 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs) = 0.93 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_{OH}* = (1.32 ± 0.19) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)
k_{OH} = 1.32 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 8.3 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988)
k_{OH} = 1.10 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, independent of temperature over the range 263–393 K (Atkinson 1989)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 6.1.5.1.1
Reported aqueous solubilities of iodobenzene at various temperatures

$$S(\mathrm{wt\%}) = -2.78956 \times 10^{-3} + 1.95862 \times 10^{-3} \cdot (t/°\mathrm{C}) - 4.53984 \times 10^{-5} \cdot (t/°\mathrm{C})^2 + 5.73315 \times 10^{-7} \cdot (t/°\mathrm{C})^3 \quad (1)$$

$$S/(\mathrm{g/kg}) = 0.59293 - 4.816 \times 10^{-3} \cdot (T/\mathrm{K}) + 1.21754 \times 10^{-5} \cdot (T/\mathrm{K})^2 \quad (2)$$

Vesala 1973		Nelson & Smit 1978		Horvath 1982		Horvath & Getzen 1985	
shake flask-UV		shake flask-GC		summary of literature data		IUPAC recommended	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
10	195.29	5	54.9	25	267.6	10	193
15.2	196.56	25	95.0	30	305.9	15	203
19.6	216.42	39	143.8	40	396.1	20	214
25.0	228.45	45.5	207.2	50	533.1	25	226
30.0	236.20					30	238
35.0	251.09			eq. 1	S/wt%	35	251
						40	264
						45	279
						eq. 2	S/(g/kg)

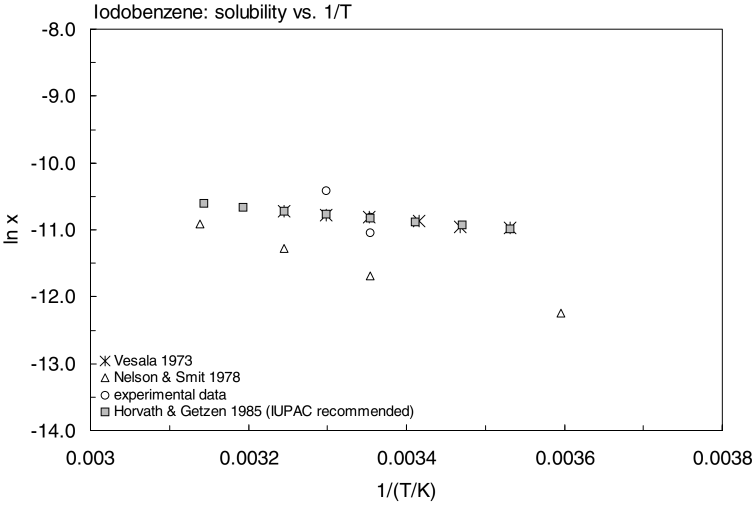


FIGURE 6.1.5.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for iodobenzene.

TABLE 6.1.5.1.2
Reported vapor pressures of iodobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Young 1889		Stull 1947	
Ramsay-Young method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
29.3	213	24.1	133.3
33	240	50.6	666.6
40.1	367	64	1333
46.3	513	78.3	2666
52.5	753	94.4	5333
57	933	105	7999
61.45	1187	118.3	13332
67.8	1627	139.8	26664
70.9	1927	163.9	53329
78.4	2700	188.6	101325
81.9	3166		
85.5	3673	mp/°C	–28.5
87.45	4026		
88.75	4266		
91.55	4820		
91.6	4820		
94.75	5466		
100.35	6919		

complete set of data see ref.

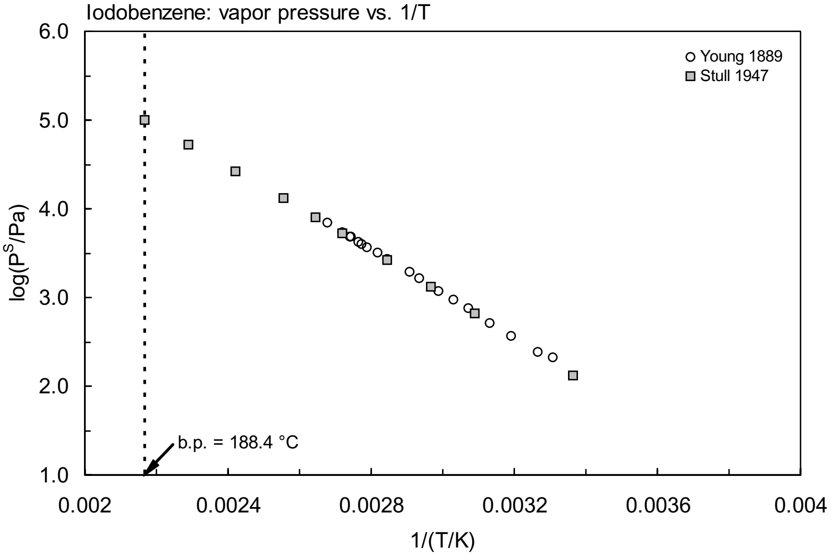
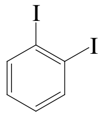


FIGURE 6.1.5.1.2 Logarithm of vapor pressure versus reciprocal temperature for iodobenzene.

6.1.5.2 1,2-Diiodobenzene



Common Name: 1,2-Diiodobenzene
Synonym: *o*-diiodobenzene
Chemical Name: 1,2-Diiodobenzene
CAS Registry No: 615-42-9
Molecular Formula: $C_6H_4I_2$
Molecular Weight: 329.051
Melting Point (°C):
27 (Weast 1982–83, Horvath 1982; Lide 2003)
Boiling Point (°C):
287 (Lide 2003)
Density (g/cm^3 at 20°C):
2.54 (20°C, Weast 1982–83, Horvath 1982; Lide 2003)
Molar Volume (cm^3/mol):
162.6 (calculated-Le Bas method at normal boiling point)
134.6 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.956 (mp at 27°C)

Water Solubility (g/m^3 or mg/L at 25°C):
14.9 (shake flask-UV, Andrews & Keefer 1950)
19.0 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
4.65 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980)
4.64 (calculated-fragment const., Yalkowsky et al. 1983)
4.65; 4.35 (quoted; calculated-molar volume correlation, Wang et al. 1992)
4.39 (calculated, Müller & Klein 1992)
4.64, 5.24; 4.56 (quoted exptl., predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

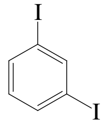
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.5.3 1,3-Diiodobenzene



Common Name: 1,3-Diiodobenzene
Synonym: *m*-diiodobenzene
Chemical Name: 1,3-Diiodobenzene
CAS Registry No: 626-00-6
Molecular Formula: $C_6H_4I_2$
Molecular Weight: 329.905
Melting Point (°C):
 40.4 (Weast 1982–83, Horvath 1982; Lide 2003)
Boiling Point (°C):
 285 (Weast 1982–83, Horvath 1982; Lide 2003)
Density (g/cm^3 at 20°C):
 2.47 (Weast 1982–83, Horvath 1982)
Molar Volume (cm^3/mol):
 162.6 (calculated-Le Bas method at normal boiling point)
 134.6 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 3.8064 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.706 (mp at 40.4°C)

Water Solubility (g/m^3 or mg/L at 25°C):
 9.67 (shake flask-UV, Andrews & Keefer 1950)
 8.88 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
 4.64 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)
 4.39 (calculated, Müller & Klein 1992)
 4.70 (calculated-molar volume correlation, Wang et al. 1992)
 5.25; 4.56 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

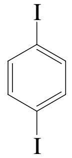
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.5.4 1,4-Diiodobenzene



Common Name: 1,4-Diiodobenzene
Synonym: *p*-diiodobenzene
Chemical Name: 1,4-Diiodobenzene
CAS Registry No: 624-38-4
Molecular Formula: $C_6H_4I_2$
Molecular Weight: 329.905
Melting Point (°C):
 131.5 (Horvath 1982; Lide 2003)
Boiling Point (°C):
 285 (sublimation, Weast 1982–83, Horvath 1982; Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
 162.6 (calculated-Le Bas method at normal boiling point)
 134.6 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 5.3342 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0902 (mp at 131.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
 4.62 (shake flask-UV, Andrews & Keefer 1950)
 1.855 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
 1.545 (extrapolated Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_S/kPa) = 8.29504 - 33311.326/(T/K)$; temp range 372–401 K (Antoine eq-I., solid, Stephenson & Malanowski 1987)
 $\log (P_L/kPa) = 6.8859 - 2747.88/(T/K)$; temp range 402–560 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
 4.64 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983; quoted, Wang et al. 1992)
 4.39 (calculated, Müller & Klein 1992)
 4.11 (shake flask, recommended, Hansch et al. 1995)
 4.64, 5.24; 4.56 (quoted exptl., predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

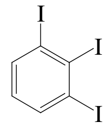
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.5.5 1,2,3-Triiodobenzene



Common Name: 1,2,3-Triiodobenzene
Synonym:
Chemical Name: 1,2,3-Triiodobenzene
CAS Registry No: 608-29-7
Molecular Formula: $C_6H_3I_3$
Molecular Weight: 455.801
Melting Point (°C):
166 (Weast 1982–83, Horvath 1982)
Boiling Point (°C):
sublimation (Weast 1982–83, Horvath 1982)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
141 (Wang et al. 1992)
195.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.041 (mp at 166°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.301 (shake flask-UV, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.86 (quoted, Wang et al. 1992)
6.17; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

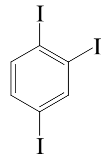
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.5.6 1,2,4-Triiodobenzene



Common Name: 1,2,4-Triiodobenzene
Synonym:
Chemical Name: 1,2,4-Triiodobenzene
CAS Registry No: 615-68-9
Molecular Formula: $C_6H_3I_3$
Molecular Weight: 455.801
Melting Point (°C):
91.5 (Weast 1982–83, Horvath 1982; Lide 2003)
Boiling Point (°C):
sublimation (Weast 1982–83, Horvath 1982; Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
195.9 (calculated-Le Bas method at normal boiling point)
145 (Wang et al. 1992)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.223 (mp at 91.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.538 (shake flask-UV, Yalowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.85 (quoted, Wang et al. 1992)
6.58; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

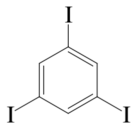
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.5.7 1,3,5-Triiodobenzene



Common Name: 1,3,5-Triiodobenzene
Synonym:
Chemical Name: 1,3,5-Triiodobenzene
CAS Registry No: 626-44-8
Molecular Formula: $C_6H_3I_3$
Molecular Weight: 455.801
Melting Point (°C):

184.2	(Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point (°C):
sublimation (Weast 1982–83, Horvath 1982; Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

131	(Wang et al. 1992)
195.9	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0274 (mp at 184.2°C)

Water Solubility (g/m^3 or mg/L at 25°C):

0.0706	(shake flask-UV, Yalowsky & Valvani 1980)
0.0644	(quoted, Wang et al. 1992)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

5.85	(quoted, Wang et al. 1992)
6.90; 5.82	(predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

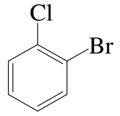
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.6 MIXED HALOGENATED BENZENES

6.1.6.1 2-Bromochlorobenzene



Common Name: 2-Bromochlorobenzene
Synonym: 2-bromo-1-chlorobenzene
Chemical Name:
CAS Registry No: 108-37-2
Molecular Formula: C_6H_4BrCl
Molecular Weight: 191.453
Melting Point (°C):
–12.3 (Weast 1982–83; Horvath 1982; Lide 2003)
Boiling Point (°C):
204 (Weast 1982–83; Horvath 1982; Lide 2003)
Density (g/cm^3):
1.6387 (25°C, Weast 1982–83; Horvath 1982)
Molar Volume (cm^3/mol):
117 (calculated-density, Lande & Banerjee 1981; Wang et al. 1992)
116.8 (Ruelle & Kesselring 1997)
140.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
124 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)
124 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
3.83 (calculated-fragment const., Yalkowsky et al. 1979)
3.86 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky 1983)
3.44 (calculated, Müller & Klein 1992)
3.83; 3.63 (quoted; calculated-molar volume correlation, Wang et al. 1992)
3.83, 3.54; 3.36 (quoted, predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

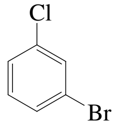
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.6.2 3-Bromochlorobenzene



Common Name: 3-Bromochlorobenzene
Synonym: *m*-bromochlorobenzene, 3-bromo-1-chlorobenzene, 1-bromo-3-chlorobenzene
Chemical Name: 3-bromochlorobenzene
CAS Registry No: 108-37-2
Molecular Formula: C_6H_4BrCl
Molecular Weight: 191.453
Melting Point (°C):
–21.5 (Dreisbach & Martin 1949, Weast 1982–83; Horvath 1982; Lide 2003)
21 (Stephenson & Malanowski 1987)
Boiling Point (C):
196 (Weast 1982–83; Horvath 1982, Stephenson & Manlanowski 1987; Lide 2003)
Density (g/cm^3):
1.62745, 1.62065 (20°C, 25°C, Dreisbach & Martin 1949)
1.602 (20°C, Weast 1982–83; Horvath 1982)
1.5771 (20°C, Lide 2003)
Molar Volume (cm^3/mol):
117.4 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
140.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
118 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)
118 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
$\log (P/mmHg) = 7.37230 - 1912.7/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
99.2 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.4972 - 1912.7/(T/K - 43.15)$; temp range 252–469 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
3.83 (calculated-fragment const., Yalkowsky et al. 1979)
3.83 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)
3.74 (HPLC-k′ correlation, Hanai et al. 1981)
3.72 (calculated, Müller & Klein 1992)
3.61 (calculated-molar volume correlation, Wang et al. 1992)
3.54; 3.36 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

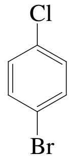
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.6.3 4-Bromochlorobenzene



Common Name: 4-Bromochlorobenzene
Synonym: 4-bromo-1-chlorobenzene, 1-bromo-4-chlorobenzene
Chemical Name: 4-bromochlorobenzene
CAS Registry No: 106-39-8
Molecular Formula: C_6H_4BrCl
Molecular Weight: 191.453
Melting Point (°C):

68	(Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point (°C):

196	(Weast 1982–83; Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

1.576	(71°C, Weast 1982–83; Horvath 1982)

Molar Volume (cm^3/mol):

121.5	(calculated-density, Stephenson & Malanowski 1987)
140.2	(calculated-Le Bas method at normal boiling point)
126.4	(Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.376 (mp at 68°C)

Water Solubility (g/m^3 or mg/L at 25°C):

44.9; 37.3	(shake flask-UV; calculated-K_{OW}, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983; quoted, Lande & Banerjee 1981; Horvath 1982; Müller & Klein 1992)
44.9; 37.3	(quoted; calculated-K_{OW}, Valvani & Yalkowsky 1980)
44.2	(quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)
45; 11.31	(quoted; calculated-molar volume correlation, Wang et al. 1992)
44.9; 50.4	(quoted; calculated-group contribution method; Kühne et al. 1995)
44.9; 51.5	(quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3*	(32.0°C, summary of literature data, temp range 32.0–196.9°C, Stull 1947)
33.3*	(24.2°C, manometry, measured range 21.4–64.4°C, Walsh & Smith 1961)
34.45	(interpolated-Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 16671.8/(T/K)] + 11.629$; temp range 23–63°C (Antoine eq., Weast 1972–73)
$\log (P/mmHg) = [-0.2185 \times 11451.1/(T/K)] + 8.222763$; temp range 32–196°C (Antoine eq., Weast 1972–73)

32.12	(calculated-bp, Mackay et al. 1982)
37.72	(interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 10.478 - 3548.4/(T/K)$; temp range 294–337 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.71377 - 2074.22/(T/K - 35.248)$; temp range 333–470 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

3.86 (calculated-fragment const., Yalkowsky et al. 1979)
3.83 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky 1983; quoted, Malihot & Peters 1988)
3.72 (calculated, Müller & Klein 1992)
3.83; 4.29 (quoted; calculated-molar volume correlation, Wang et al. 1992)
3.83, 3.73; 3.36 (quoted, predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

TABLE 6.1.6.3.1
Reported vapor pressures of 4-bromochlorobenzene at various temperatures

Stull 1947		Walsh & Smith 1961	
summary of literature data		manometry	
t/°C	P/Pa	t/°C	P/Pa
32.0	133.3	21.4	22.7
59.5	666.6	24.2	33.3
72.7	1333	26.1	37.3
87.8	2666	29.0	53.3
103.8	5333	30.7	58.7
114.8	7999	35.4	96.0
128.0	13332	35.6	93.3
149.5	26664	40.5	144.0
172.6	53329	40.6	144.0
196.9	101325	44.5	200.0
		45.6	221.3
		48.9	284
		49.9	313.3
		53.0	401.3
		54.7	457.3
		57.1	545.3
		59.9	673.3
		60.7	710.6
		64.0	902.6
		64.4	911.9

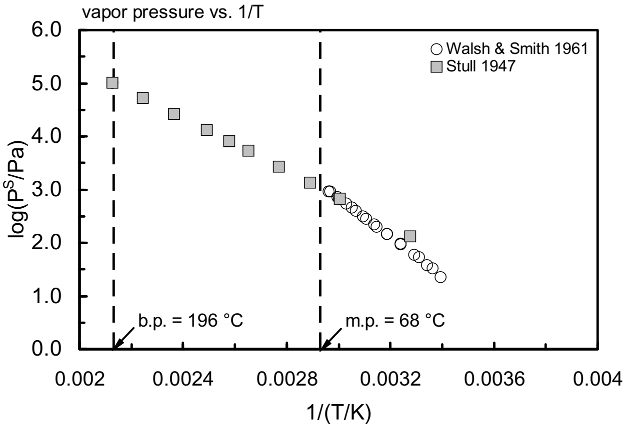
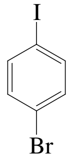


FIGURE 6.1.6.3.1 Logarithm of vapor pressure versus reciprocal temperature for 4-bromochlorobenzene.

6.1.6.4 4-Bromoiodobenzene



Common Name: 4-Bromoiodobenzene
Synonym: 4-bromo-1-iodobenzene
Chemical Name:
CAS Registry No: 589-87-7
Molecular Formula: C_6H_4BrI
Molecular Weight: 282.904
Melting Point (°C):

92	(Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point (°C):

252	(Weast 1982–83; Horvath 1982, Lide 2003)

Density (g/cm^3):

2.235	(Weast 1982–83; Horvath 1982; Lide 2003)

Molar Volume (cm^3/mol):

152.6	(calculated-Le Bas method at normal boiling point)
128.1	(Rulle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.13	(Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.22 (mp at 92°C)

Water Solubility (g/m^3 or mg/L at 25°C):

7.8	(shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980, Valvani & Yalkowsky 1980)
7.94	(quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

4.36	(calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)
4.62; 4.10	(predicted; calculated-atom typing scheme, Onel & Iseri 1997)
4.13	(calculated, Müller & Klein 1992)

Octanol/Air Partition Coefficient, log K_{OA}:

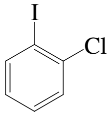
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

6.1.6.5 2-Chloroiodobenzene



Common Name: 2-Chloroiodobenzene
Synonym: 2-chloro-1-iodobenzene
Chemical Name:
CAS Registry No: 615-41-8
Molecular Formula: ClC_6H_4I
Molecular Weight: 238.453
Melting Point (°C):

0.7	(Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point (°C):

234.5	(Weast 1982–83; Horvath 1982; Lide 2003)

Density (g/cm^3):

1.9515	(Weast 1982–83; Horvath 1982)
1.9255	(20°C, Lide 2003)

Molar Volume (cm^3/mol):

150.2	(calculated-Le Bas method at normal boiling point)
134.6	(Rulle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

68.8	(shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
68.68	(quoted, Horvath 1982; IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

4.12	(calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)
3.98	(calculated, Müller & Klein 1992)
2.54; 3.89	(quoted; calculated-molar volume correlation, Wang et al. 1992)
4.05, 3.82	(predicted; calculated-atom typing scheme, Onel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

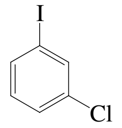
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.6.6 3-Chloroiodobenzene



Common Name: 3-Chloroiodobenzene
Synonym: 3-chloro-1-iodobenzene
Chemical Name:
CAS Registry No: 625-99-0
Molecular Formula: ClC_6H_4I
Molecular Weight: 238.453
Melting Point (°C):
Boiling Point (°C):

230	(Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.9515	(25°C, Weast 1982–83)
1.9255	(20°C, Horvath 1982)

Molar Volume (cm^3/mol):

150.2	(calculated-Le Bas method at normal boiling point)
124.9	(Rulle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

68.8	(shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
67.4	(quoted, Horvath 1982; IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

4.12	(calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)
4.05, 3.82	(predicted; calculated-atom typing scheme, Onel & Iseri 1997)
3.98	(calculated, Müller & Klein 1992)

Octanol/Air Partition Coefficient, log K_{OA}:

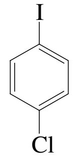
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.6.7 4-Chloroiodobenzene



Common Name: 4-Chloroiodobenzene
Synonym: 4-chloro-1-iodobenzene
Chemical Name:
CAS Registry No: 637-87-6
Molecular Formula: ClC_6H_4I
Molecular Weight: 238.453
Melting Point (°C):
  57 (Weast 1982–83; Horvath 1982; Lide 2003)
Boiling Point (°C):
  227 (Weast 1982–83; Horvath 1982; Lide 2003)
Density (g/cm^3):
  1.886 (57°C, Weast 1982–83; Horvath 1982)
Molar Volume (cm^3/mol):
  122 (calculated-density, Lande & Banerjee 1981)
  126.4 (Stephenson & Malanowski 19987; Rulle & Kesselring 1997)
  127 (Wang et al. 1992)
  150.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.4825

Water Solubility (g/m^3 or mg/L at 25°C):
  22.5 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
  31.11 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  16.26 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_S/kPa) = 8.944 - 3200/(T/K)$; temp range 303–323 K (Antoine eq.-I, solid state, Stephenson & Malanowski 1987)
  $\log (P_L/kPa) = 5.63678 - 1465.651/(T/K - 102.487)$; temp range 333–500 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):k′

Octanol/Water Partition Coefficient, log K_{OW}:
  4.12 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky)
  4.06 (HPLC-k′ correlation, Hanai et al. 1981)
  3.98 (calculated, Müller & Klein 1992)
  4.47 (calculated-molar volume correlation, Wang et al. 1992)
  4.34; 3.82 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:

6.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 6.2.1
Summary of physical properties of chlorobenzenes and other halogenated mononuclear aromatics

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/cm³ at 20°C	Molar volume, V_M cm³/mol	
								from ρ$^{(a)}$	Le Bas
Chlorobenzenes:									
Chlorobenzene	108-90-7	C_6H_5Cl	112.557	–45.31	131.72	1	1.1058	101.79	116.9
1,2-Dichloro-	95-50-1	$C_6H_4Cl_2$	147.002	–17.0	180	1	1.3059	112.57	137.9
1,3-Dichloro-	541-73-1	$C_6H_4Cl_2$	147.002	–24.8	173	1	1.2884	114.10	137.8
1,4-Dichloro-	106-46-7	$C_6H_4Cl_2$	147.002	53.09	174	0.530	1.2457	118.01	137.8
1,2,3-Trichloro-	87-61-6	$C_6H_3Cl_3$	181.447	51.3	218.5	0.552		125‡	158.7
1,2,4-Trichloro-	120-82-1	$C_3H_3Cl_3$	181.447	16.92	213.5	1	1.4542	124.77	158.7
1,3,5-Trichloro-	108-70-3	$C_6H_3Cl_3$	181.447	62.8	208	0.426		125‡	158.7
1,2,3,4-Tetrachloro-	634-66-2	$C_6H_2Cl_4$	215.892	47.5	254	0.602		142‡	179.6
1,2,3,5-Tetrachloro-	634-90-2	$C_6H_2Cl_4$	215.892	54.5	246	0.514		142‡	179.6
1,2,4,5-Tetrachloro-	95-94-3	$C_6H_2Cl_4$	215.892	139.5	244.5	0.0753		142‡	179.6
Pentachlorobenzene	608-93-5	C_6HCl_5	250.337	86	277	0.252		166‡	200.5
Hexachlorobenzene	118-74-1	C_6Cl_6	284.782	228.83	325	0.0100		186‡	221.4
Chlorotoluenes:									
2-Chlorotoluene	95-49-8	C_7H_7Cl	126.584	–35.8	159.0	1	1.0825	116.94	139.1
3-Chlorotoluene	108-41-8	C_7H_7Cl	126.584	–47.8	161.8	1	1.0722	118.06	139.1
4-Chlorotoluene	106-43-4	C_7H_7Cl	126.584	7.5	162.4	1	1.0697	118.34	139.1
2,4-Dichlorotoluene	95-73-8	$C_7H_6Cl_2$	161.029	–13.5	201	1	1.2476	129.07	160.0
2,6-Dichlorotoluene	118-69-4	$C_7H_6Cl_2$	161.029	25.8	198	1	1.2686	126.93	160.0
3,4-Dichlorotoluene	95-75-0	$C_7H_6Cl_2$	161.029	–15.2	208.9	1	1.2564	128.17	160.0
2,3,6-Trichlorotoluene	2077-46-5	$C_7H_5Cl_3$	195.474	45.5	229.5	0.629			180.9
2,4,5-Trichlorotoluene	6639-30-1	$C_7H_5Cl_3$	195.474	82.4	231	0.273			180.9
α-Chlorotoluene	100-44-7	C_7H_7Cl	126.584	–45	179	1	1.1004	115.03	139.1
α, α, α-Trichlorotoluene	98-07-7	$C_7H_5Cl_3$	195.474	–4.42	221	1	1.3723	142.44	180.9
Pentachlorotoluene	877-11-2	$C_7H_3Cl_5$	264.364	224.8	301	0.0110			222.7
o-Chlorostyrene	2039-87-4	C_8H_7Cl	138.595	–63.1	188.7	1	1.1000	126.00	153.9
m-Chlorostyrene	2039-85-2	C_8H_7Cl	138.595				1.1033	125.62	153.9
p-Chlorostyrene	1073-67-2	C_8H_7Cl	138.595	15.9	192	1	1.0868	127.53	153.9
Octachlorostyrene	29082-74-4	C_8Cl_8	379.710	99		0.188			300.2

(Continued)

TABLE 6.2.1 (*Continued*)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/cm³ at 20°C	Molar volume, V_M cm³/mol	
								from ρ[(a)]	Le Bas
Fluorobenzenes:									
Fluorobenzene	462-06-6	C_6H_5F	96.102	-42.18	84.73	1	1.0225	93.99	101.0
1,2-Difluorobenzene	367-11-3	$C_6H_4F_2$	114.093	–47.1	94	1	1.158	98.53	106.0
1,3-Difluorobenzene	372-18-9	$C_6H_4F_2$	114.093	–69.12	82.6	1	1.1572	98.59	106.0
1,4-Difluorobenzene	540-36-3	$C_6H_4F_2$	114.093	–23.55	89	1	1.1701	97.51	106.0
1,2,4-Trifluorobenzene	367-23-7	$C_6H_3F_3$	132.083		90	1			111.0
1,3,5-Trifluorobenzene	372-38-3	$C_6H_3F_3$	132.083	–5.5	75.5	1		103.4†	111.0
1,2,3,4-Tetrafluorobenzene	551-62-2	$C_6H_2F_4$	150.074		94.3	1		105.5†	116.0
1,2,3,5-Tetrafluorobenzene	2367-82-0	$C_6H_2F_4$	150.074	–46.25	84.4	1		107.7†	116.0
1,2,4,5-Tetrafluorobenzene	327-54-8	$C_6H_2F_4$	150.074	3.88	90.2	1	1.4255	105.28	116.0
Pentafluorobenzene	363-72-4	C_6HF_5	168.064	–47.4	85.74	1		111.0†	121.0
Hexafluorobenzene	392-56-3	C_6F_6	180.054	5.03	80.26	1	1.6184	111.25	126.0
Pentafluorotoluene	771-56-2	$C_7H_3F_5$	182.091	–29.78	117.5	1	1.440	126.45	143.2
Chloropentafluorobenzene	344-07-0	C_6ClF_5	202.509		117.96				141.9
Pentafluorophenol	771-61-9	C_6HF_50	184.063	37.5	145.6	0.754			128.4
Bromobenzenes and bromotoluenes:									
Bromobenzene	108-86-1	C_6H_5Br	157.008	–30.72	156.06	1	1.4950	105.02	119.3
1,2-Dibromobenzene	583-53-9	$C_6H_4Br_2$	235.904	7.1	225	1	1.9843	118.89	142.6
1,3-Dibromobenzene	108-36-1	$C_6H_4Br_2$	235.904	–7.0	218	1	1.9523	120.83	142.6
1,4-Dibromobenzene	106-37-6	$C_6H_4Br_2$	235.904	87.43	218.5	0.244	1.5742	149.86	142.6
1,2,3-Tribromobenzene	608-21-9	$C_6H_3Br_3$	314.800	87.8		0.242	2.6580	118.43	165.9
1,2,4-Tribromobenzene	615-54-3	$C_6H_3Br_3$	314.800	44.5	275	0.644			165.9
1,3,5-Tribromobenzene	626-39-1	$C_6H_3Br_3$	314.800	122.8	271	0.110			165.9
1,2,4,5-Tetrabromobenzene	636-28-2	$C_6H_2Br_4$	393.696	182		0.0288	3.0720	128.16	189.2
Hexabromobenzene	87-82-1	C_6Br_6	551.488	327		0.0011			235.8
2-Bromotoluene	95-46-5	C_7H_7Br	171.035	–27.8	181.7	1	1.4232	120.18	141.5
3-Bromotoluene	591-17-3	C_7H_7Br	171.035	–39.8	183.7	1	1.4099	121.31	141.5
4-Bromotoluene	106-38-7	C_7H_7Br	171.035	28.5	184.3	1			141.5
Iodobenzenes:									
Iodobenzene	591-50-4	C_6H_5I	204.008	–31.3	188.4	1	1.8308	111.43	129.3
1,2-Diiodobenzene	615-42-9	$C_6H_4I_2$	329.905	27	287	0.956	2.5400	129.88	162.6
1,3-Diiodobenzene	626-00-6	$C_6H_4I_2$	329.905	40.4	285	0.706			162.6
1,4-Diiodobenzene	624-38-4	$C_6H_4I_2$	329.905	131.5	285	0.0902			162.6

1,2,3-Triiodobenzene	608-29-7	$C_6H_3I_3$	455.801	166	sublim	0.0410		141§	195.9
1,2,4-Triiodobenzene	615-68-9	$C_6H_3I_3$	455.801	91.5	sublim	0.223		145§	195.9
1,3,5-Triiodobenzene	626-44-8	$C_6H_3I_3$	455.801	184.2	sublim	0.0274		131§	195.9
Mixed halogenated benzenes:									
2-Bromochlorobenzene	694-80-4	C_6H_4BrCl	191.453	–12.3	204	1		117§	140.2
3-Bromochlorobenzene	108-37-2	C_6H_4BrCl	191.453	–21.5	196	1	1.5771	121.40	140.2
4-Bromochlorobenzene	106-39-8	C_6H_4BrCl	191.453	68	196	0.379		121.5†	140.2
4-Bromoiodobenzene	589-87-7	C_6H_4BrI	282.904	92	252	0.220	2.2350	126.58	152.6
2-Chloroiodobenzene	615-41-8	ClC_6H_4I	238.453	0.7	234.5	1	1.9255	123.84	150.2
3-Chloroiodobenzene	625-99-0	ClC_6H_4I	238.453		230	1	1.9255	123.84	150.2
4-Chloroiodobenzene	637-87-6	ClC_6H_4I	238.453	57	227	0.485		127§	150.2

* Assuming ΔS_{fus} = 56 J/mol K

(a) † Chiou 1985 (liquid molar volume), † Stephenson & Malanowski 1987, §Wang et al. 1992, and calculated as MW/ρ at 20°C for this work

TABLE 6.2.2
Summary of selected physical-chemical properties of chlorobenzenes and other halogenated mononuclear aromatics at 25°C

	Selected properties						Henry's law constant
	Vapor pressure		Solubility				
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}	H/(Pa·m³/mol) calculated P/C
Chlorobenzenes:							
Chlorobenzene	1580	1580	484	4.3000	4.2300	2.80	367
1,2-Dichloro-	170	170	140	0.9523	0.9523	3.40	178
1,3-Dichloro-	260	260	120	0.8163	0.8163	3.40	318
1,4-Dichloro-	130	245	80	0.544	1.0268	3.40	242
1,2,3-Trichloro-	28	50.72	21	0.1157	0.2100	4.10	242
1,2,4-Trichloro-	40	40	40	0.2204	0.2204	4.10	277
1,3,5-Trichloro-	25	78.05	5.3	0.0292	0.0686	4.10	856
1,2,3,4-Tetrachloro-	4.0	6.64	7.8	0.0361	0.0600	4.50	111
1,2,3,5-Tetrachloro-	9.8	19.01	3.6	0.0167	0.0324	4.50	588
1,2,4,5-Tetrachloro-	0.72	9.56	1.27	0.00588	0.0781	4.50	122
Pentachlorobenzene	0.22	0.8730	0.65	0.00260	0.0103	5.00	85
Hexachlorobenzene	0.0023	0.23	0.005	0.0000176	0.00176	5.50	131

TABLE 6.2.3
Suggested half-life classes of chlorobenzenes and other halogenated mononuclear aromatics in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Chlorobenzene	4	6	7	8
1,2-Dichloro-	5	6	7	8
1,3-Dichloro-	5	6	7	8
1,4-Dichloro-	5	6	7	8
1,2,3-Trichloro-	5	6	7	8
1,2,4-Trichloro-	5	6	7	8
1,3,5-Trichloro-	5	6	7	8
1,2,3,4-Tetrachloro-	6	7	7	8
1,2,3,5-Tetrachloro-	6	7	7	8
1,2,4,5-Tetrachloro-	6	7	7	8
Pentachlorobenzene	7	8	8	8
Hexachlorobenzene	8	9	9	9
Fluorobenzene	4	5	6	7
Bromobenzene	4	6	7	8
Iodobenzene	4	6	7	8

where,

Class	Mean half-life (hours)	Range (hours)
1	5	<10
2	17 (~1 day)	10–30
3	55 (~2 days)	30–100
4	170 (~1 week)	100–300
5	550 (~3 weeks)	300–1,000
6	1,700 (~2 months)	1,000–3,000
7	5,500 (~8 months)	3,000–10,000
8	17,000 (~2 years)	10,000–30,000
9	55,000 (~6 years)	>30,000

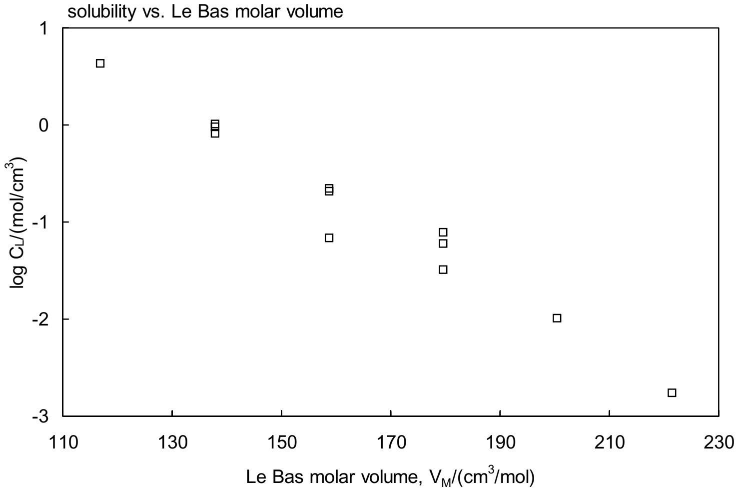


FIGURE 6.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for chlorobenzenes.

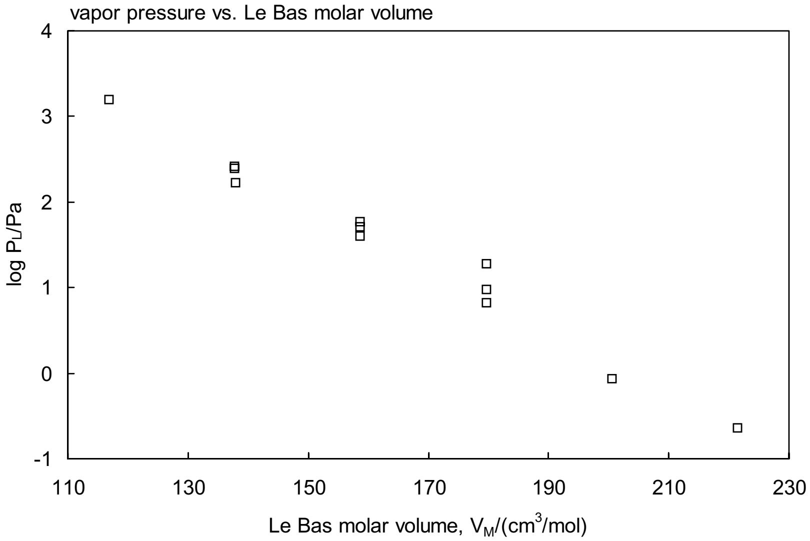


FIGURE 6.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for chlorobenzenes.

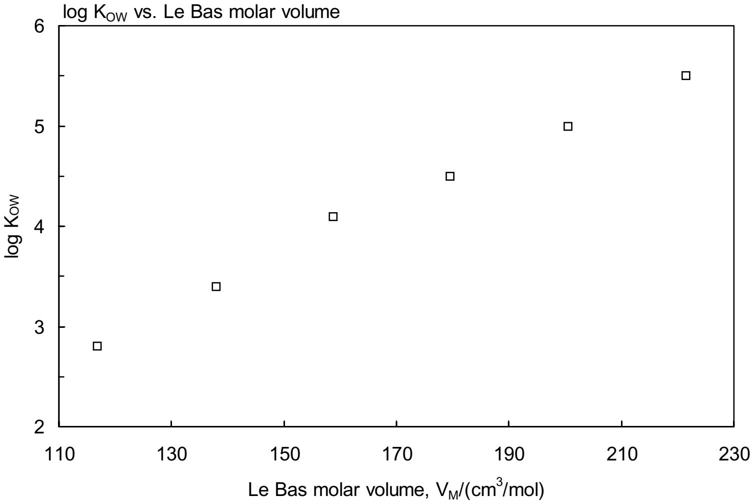


FIGURE 6.2.3 Octanol-water partition coefficient versus Le Bas molar volume for chlorobenzenes.

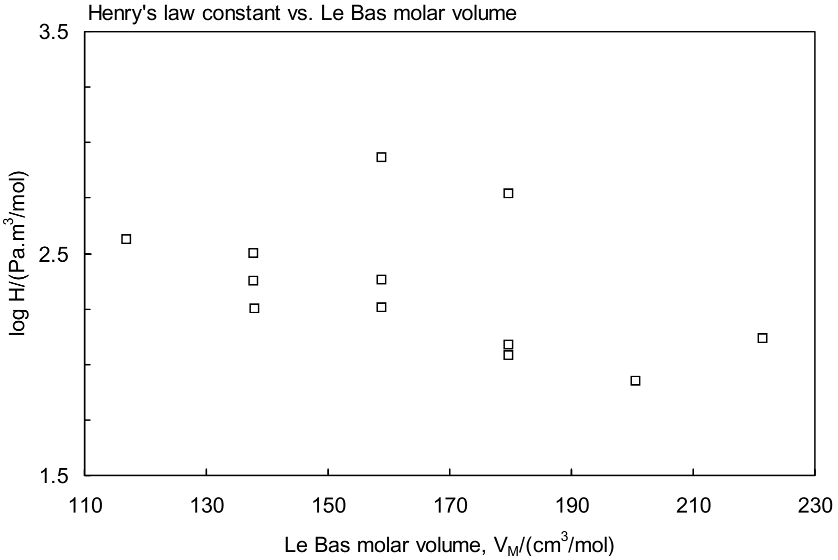


FIGURE 6.2.4 Henry's law constant versus Le Bas molar volume for chlorobenzenes.

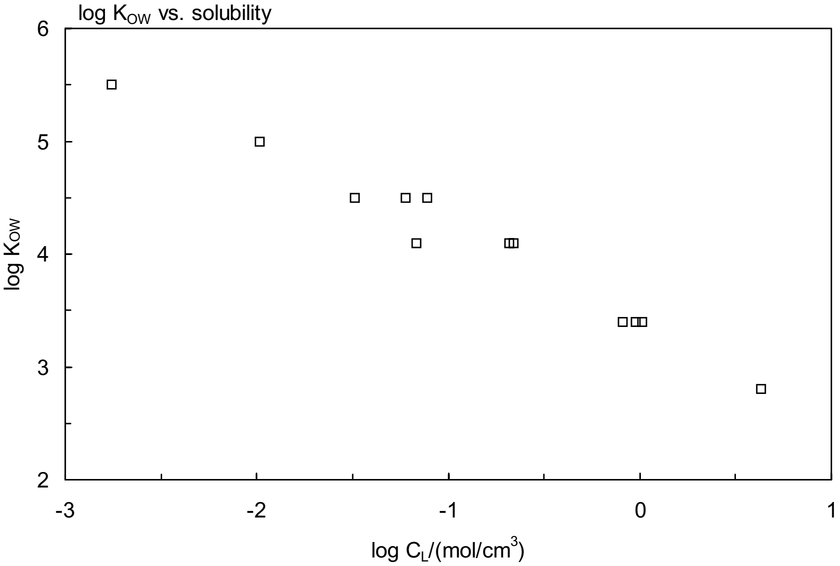


FIGURE 6.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) chlorobenzenes.

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7 Polychlorinated Biphenyls (PCBs)

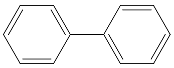
CONTENTS

7.1 LIST OF CHEMICALS AND DATA COMPILATIONS

7.1.1 PCB CONGENERS

7.1.1.0 Biphenyl

(See also Chapter 4, Polynuclear Aromatic Hydrocarbons [PAHs] and Related Aromatic Hydrocarbons)



Common Name: Biphenyl
Synonym: diphenyl, phenylbenzene
Chemical Name: biphenyl
CAS Registry No: 92-52-4
Molecular Formula: $C_{12}H_{10}$
Molecular Weight: 154.207
Melting Point (°C):
  68.93 (Lide 2003)
Boiling Point (°C):
  256.1 (Lide 2003)
Density (g/cm^3 at 20°C):
  0.866 (20°C, Weast 1982–1983)
  1.04 (Lide 2003)
Molar Volume (cm^3/mol):
  148.3 (20°C, calculated-density)
  184.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  18.58 (Parks & Huffman 1931)
  18.66 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  51.05 (Miller et al. 1984)
  54.81, 59.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.371 (mp at 68.93°C)
  0.35 (Mackay et al. 1980,1983; Shiu & Mackay 1986; Shiu et al. 1987)
  0.381 (calculated, ΔS_{fus} = 54 J/mol K, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  5.94 (shake flask-UV, Andrews & Keefer 1949)
  7.48* (shake flask-UV, measured range 0.4–42.8°C, Bohon & Claussen 1951)
  3.87 (shake flask-UV, Sahyun 1966)
  7.08* (shake flask-UV, measured range 0–64.5°C, Wauchope & Getzen 1972)
  $R \cdot \ln x = -4520/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 298.15]^2 - 20.8 + 0.0273 \cdot (T/K)$, temp range 24.6–73.4°C (shake flask-UV measurements, Wauchope & Getzen 1972)
  7.45 (shake flask-GC, Eganhouse & Calder 1976)
  7.0 (shake flask-fluorescence, Mackay & Shiu 1977)
  8.50 (shake flask-nephelometry, Hollifield 1979)
  7.51 (shake flask-LSC, Banerjee et al. 1980)
  8.09 (TLC-RT correlation, Bruggeman et al. 1982)
  6.71 (generator column-GC/ECD, Miller et al. 1984, 1985; quoted, Hawker 1989b)
  7.09 (recommended, Pearlman et al. 1984)
  7.05 (vapor saturation-UV, Akiyoshi et al. 1987)
  6.5 (29°C, shake flask-GC/FID; Stucki & Alexander 1987)
  7.20, 7.55 (generator column-HPLC/UV, Billington et al. 1988)

9.96, 9.96, 9.96, 10.67 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.2* (recommended, IUPAC Solubility Data Series, Shaw 1989)

log [S_L/(mol/L)] = 1.872 –973.4/(T/K) (supercooled liquid, Passivirta et al. 1999)

ln x = –1.5792 – 3669.26/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

5.37, 5.32 (generator column-GC/ECD, different flow rates, Oleszek-Kudlak et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7933* (162.5°C, isoteniscope-manometer, measured range 162.5–255.2°C, Chipman & Peltier 1929)

104* (69.20°C, temp range 69.20–271.2°C, Cunningham 1930; quoted, Boublik et al. 1984)

133.3* (70.6°C, summary of literature data, temp range 70.6–254.0°C, Stull 1947)

1.30 (effusion method, measured range 4.0–34.5°C, Bright 1951)

log (P/mmHg) = 10.38 – 3799/(T/K); temp range: 4.0–34.5°C (Antoine eq., effusion, Bright 1951)

0.031 (manometry, Augood et al. 1953; selected, Bidleman 1984)

1.273* (effusion method, measured range 15.05–40.55°C, Bradley & Cleasby 1953)

log (P/cmHg) = 11.282 – 4263/(T/K); temp range 15.05–40.55°C (Antoine eq., Bradley & Cleasby 1953)

log (P/mmHg) = [– 0.2185 × 12910.0/(T/K)] + 8.218583; temp range 70.6–254.9°C (Antoine eq., Weast 1972–73)

1.41* (effusion method, interpolated-Antoine eq., measured range 24.9–50.33°C, Radchenko & Kitiagorodskii 1974)

log (P/mmHg) = 12.6789 – 4367.436/(T/K); temp range; 24.9–50.33°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)

2040* (123.0°C, pressure transducer, measured range 123.0–327.55°C, Nasir et al. 1980)

1.40 (HPLC-RT correlation, Swann et al. 1983)

log (P/atm) = $[1 - 528.437/(T/K)] \times 10^{\wedge}\{0.821410 - 2.73337 \times 10^{-4} \cdot (T/K) + 1.02285 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 342.35–673.15 K (Cox eq., Chao et al. 1983)

3.35, 3.41 (P_{GC} by GC-RT correlation, different GC columns, Bidleman 1984)

5.608 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)

log (P/kPa) = 6.36895 – 1997.558/(202.608 + t/°C), temp range: 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.15* (24.7°C, gas saturation-GC/FID, measured range 5.2–24.7°C, Burkhard et al. 1984)

log (P/Pa) = 14.840 – 4402.1/(T/K), temp range: 5.2–24.7°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)

2.03 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)

log (P/mmHg) = 7.24541 – 1998.725/(202.733 + t/°C), temp range: 69–271°C (Antoine eq., Dean 1985, 1992)

5.61; 6.62 (supercooled liquid P_L, quoted lit.; GC-RT correlation, Foreman & Bidleman 1985)

2.43; 6.90 (selected P_S; supercooled liq. P_L, Shiu & Mackay 1986; Shiu et al. 1987; Sklarew & Girvin 1987)

1.443; 1.23 (P_S, interpolated-Antoine equations; Stephenson & Malanowski 1987)

log (P_S/kPa) = 11.71929 – 4143.054/(T/K); temp range 297–324 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_S/kPa) = 28.5175 – 21141.5/(374.85 + T/K); temp range: 283–342 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.37526 – 1794.8/(– 74.85 + T/K), temp range: 390–563 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

5.10, 5.00 (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)

3.35 (P_{GC} by GC-RT correlation, Hinckley et al. 1990)

0.422–2.54; 2.03–7.04(quoted range of lit. P_S values; lit. P_L values, Delle Site 1997)

5.31; 2.02 (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

log (P_S/Pa) = 11.05 – 3201/(T/K) (solid, Passivirta et al. 1999)

log (P_L/Pa) = 8.20 – 2228/(T/K) (supercooled liquid, Passivirta et al. 1999)

log (P/kPa) = 14.840 – 4402.1/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

3.63; 0.822 (supercooled liquid P_L, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

log (P_L/Pa) = – 3265/(T/K) + 11.51; $\Delta H_{vap.}$= – 62.5 kJ·mol^{-1} (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

41.34 (batch stripping-GC, Mackay et al. 1979)
30.4 (batch stripping-GC, Mackay et al. 1980;)
11.55 (gas stripping-GC, Warner et al. 1987)
19.57 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
31.20 (gas stripping-GC, Shiu & Mackay 1997)
$\log [H/(Pa\ m^3/mol)] = 6.33 - 1255/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:

3.16 (shake flask-UV, Rogers & Cammarata 1969)
4.09 (shake flask, Leo et al. 1971; Hansch & Leo 1979)
4.04 (shake flask, Hansch et al. 1973)
4.17, 4.09, 3.16, 4.04 (Neely et al. 1974; Hansch & Leo 1979)
3.95 (HPLC-k′ correlation, Rekker & De Kort 1979)
3.75 (HPLC-RT correlation, Veith et al. 1979a)
4.04 (shake flask-HPLC, Banerjee et al. 1980)
3.88 (lit. average, Kenaga & Goring 1980)
4.10 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
4.08 (HPLC-k′ correlation, Hammers et al. 1982)
3.70 (HPLC-RT correlation, Woodburn 1982; Woodburn et al, 1984)
3.16–4.09, 3.91 (shake flask, range, average, Eadsforth & Moser, 1983)
3.91–4.15, 4.05 (HPLC, range, average, Eadsforth & Moser 1983)
4.03 (HPLC-k′ correlation, Hafkenscheid & Tomlinson 1983)
3.93 (HPLC correlation; Harnisch et al. 1983)
3.76 (generator column-GC/ECD, Miller et al. 1984,1985)
3.89 (generator column-HPLC, Woodburn et al. 1984)
3.79 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.11–4.13 (HPLC-RV correlation, quoted exptl., Garst 1984)
4.10 (HPLC-RV correlation, Garst & Wilson 1984)
4.05 (HPLC-RT correlation, Eadsforth 1986)
3.81 (shake flask-GC, Menges & Armstrong 1986)
4.13 (HPLC-RT correlation, Wang et al. 1991)
3.63 (HPLC-k′ correlation; De Kock & Lord 1987)
3.89 (generator column-GC, Doucette & Andren 1987,1988)
4.14, 4.06, 4.00, 3.94 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.69 (HPLC-RT correlation, Doucette & Andren 1988)
3.75 (HPLC-RT correlation, Sherblom & Eganhouse 1988)
4.008; 4.10 (slow stirring-GC; calculated-π const., De Bruijn et al. 1989; De Bruijn & Hermens 1990)
3.98 (recommended, Sangster 1989, 1993)
4.29 (dual-mode centrifugal partition chromatography, Gluck & Martin 1990)
4.26 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

6.92, 6.09; 6.09 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
6.15 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

2.64 (trout, calculated-k_1/k_2, Neely et al. 1974)
3.12 (rainbow trout, Veith et al. 1979; Veith & Kosian 1983)
2.53 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
2.73, 2.45, 3.41 (algae, fish, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

3.15 (soil, Kenaga 1980)
3.0, 3.27 (Aldrich humic acid, reversed phase separation, Landrum et al. 1984)
3.57, 3.77 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with 9.6 mg/L DOC, Landrum et al. 1984)
5.58, 4.04 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 mg/L DOC, Landrum et al. 1984)
5.68, 5.34, 5.23, 3.57 (humic materials in natural water: Huron River 6.7% DOC spring, Grand River 10.7% DOC spring, Lake Michigan 4.7% DOC spring, Lake Erie 9.6% DOC spring, RP-HPLC separation method, Landrum et al. 1984)
3.52, 2.94 (Apison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium, Southworth & Keller 1986)
3.40 (calculated, soil, Chou & Griffin 1986)
3.04, 3.32, 3.26, 3.04, 3.08 (5 soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
4.20; 3.30 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
3.03, 3.12 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average values, Delle Site 2001)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization/Evaporation: $t_{½}$ = 7.52 d evaporation from water depth of 1 m (Mackay & Leinonen 1975)
rate of volatilization k = 0.92 g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis: k = 5.1×10^{-4} h^{-1} to 7.4×10^{-3} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988);
photodegradation k = 5.1×10^{-4} min^{-1} and $t_{½}$ = 22.61 h in methanol-water (3:7, v/v) with initial concentration of 16.2 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH} = $(8.06 \pm 0.77) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with an estimated lifetime of ~3 d, and k_{O3} < 2.0×10^{-19} cm^3 $molecule^{-1}$ s^{-1} at 294 ± 1 K (relative rate method, Atkinson et al. 1984)
k_{OH} = $(8.5 \pm 0.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1985)
k_{OH} = $(7 \pm 2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1985)
k_{OH}(calc) = 7.9×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = $(5.8 - 8.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 3 d (Atkinson 1987a)
k_{OH}(calc) = 7.1×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 7.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (SAR structure-activity relationship, Atkinson 1987b)
k_{O3} < 2×10^{-19} cm^3 $molecule^{-1}$ s^{-1}; k_{OH} = 7.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1}; k_{N2O5} < 2.0×10^{-19} cm^3 $molecule^{-1}$ s^{-1} for reaction with N_2O_5 at room temp (Atkinson & Aschmann 1988)
k_{OH}* = 7.2×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
k_{OH}(calc) = 6.44×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)
k_{OH}(exptl) = 7.2×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 6.7×10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 2.0 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 100% degraded by activated sludge in 47 h cycle (Monsanto Co. 1972)
k = 109 yr^{-1} in the water column and k = 1090 yr^{-1} in the sediment, microbial degradation pseudo first-order rate constant (Wong & Kaiser 1975; selected, Neely 1981)
k = 9.3–9.8 nmol L^{-1} d^{-1} with an initial biphenyl concentration of 4.4–4.7 μmol/L, and k = 3.2 nmol L^{-1} d^{-1} with initial concentration of 2.9 μmol/L, rate of biodegradation in water from Port Valdez (estimated, Reichardt et al. 1981)
$t_{½}$ = 1.5 d, estimated by using water die-away test (Bailey et al. 1983)
$t_{½}$(aq. aerobic) = 36–168 h, based on river die-away test data and activated sludge screening test data (Howard et al. 1991)
$t_{½}$(aq. anaerobic) = 144–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

removal rate of 5.3 and 0.52 mg (g of volatile suspended solid d)$^{-1}$, degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

k_1 = 6.79 h^{-1}; k_2 = 0.0155 h^{-1} (trout muscle, Neely et al. 1974; Neely 1979)

k_1 = 6.8 h^{-1}; $1/k_2$ = 65 h (trout, quoted, Hawker & Connell 1985)

log k_1 = 2.21 d^{-1}; log $1/k_2$ = 0.43 d (fish, Connell & Hawker 1988)

log k_2 = – 0.43 d^{-1} (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air: calculated lifetime of ~3 d due to reaction with OH radical, assuming an average daytime atmospheric OH radical concn of ~1×10^6 molecule/cm^3 (Atkinson et al. 1984);

estimated atmospheric lifetime of ~2.7 d due to reaction with the OH radical for a 24-h average OH radical concn of 5×10^5 cm^{-3} (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 9 d due to the rate constants of gas-phase reaction with OH radical (Atkinson 1987);

$t_{1/2}$ = 7.8–110 h, based on photooxidation half-life in air (Howard et al. 1991);

tropospheric lifetime of 2.0 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for biphenyl (Kwok et al. 1995).

Surface water: $t_{1/2}$ ~1.5 d in river water (Bailey et al. 1983);

$t_{1/2}$ = 36–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

photolysis $t_{1/2}$ = 19.18 min in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2}$ = 72–336 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2}$ = 36–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota: estimated $t_{1/2}$ = 29 h from fish in simulated ecosystem (Neely 1980).

TABLE 7.1.1.0.1
Reported aqueous solubilities of biphenyl at various temperatures:

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
			experimental		smoothed		
0.40	2.83	24.6	7.13	0	2.64	0	2.72
2.4	2.97	24.6	7.29	24.6	6.96	10	4.1
5.2	3.38	24.6	7.35	25	7.08	20	6.3
7.6	3.64	29.9	8.77	29.9	8.73	25	7.2
10	4.06	29.9	8.64	30.3	8.88	30	9.1
12.6	4.58	29.9	895	38.4	12.7	40	14.4
14.9	5.11	30.3	8.55	40.1	13.8	50	22
15.9	5.27	30.3	8.54	47.5	19.5	69	37
25	7.48	30.3	8.48	50	22.0		
25.6	7.78	38.4	13.2	50.1	22.1		
30.1	9.64	38.4	13.3	50.2	22.2		
30.4	9.58	38.4	13.5	54.7	27.7		
33.3	11.0	40.1	13.1	59.2	34.8		
34.9	11.9	40.1	13.4	60.5	37.2		
36	12.5	40.1	13.4	64.5	45.9		
42.8	17.2	47.5	18.8				
		47.5	19.0	temp dependence eq. 1			

TABLE 7.1.1.0.1 (*Continued*)

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	$S/g{\cdot}m^{-3}$	t/°C	$S/g{\cdot}m^{-3}$	t/°C	$S/g{\cdot}m^{-3}$	t/°C	$S/g{\cdot}m^{-3}$
for supercooled liquid:		47.5	18.7	ln *x*	mole fraction		
$\Delta H_{sol}/(kJ\ mol^{-1})$ =		50.1	20.6	ΔH_{fus}	18.9 ± 0.50		
at 275 K	7.03	50.1	21.6	$10^2{\cdot}b$	2.73 ± 0.12		
280 K	10.13	50.1	21.8	c	20.8 ± 0.4		
285 K	11.25	50.2	20.7				
290 K	12.55	50.2	21.8				
295 K	13.43	54.7	28.3				
300 K	15.02	54.7	28.8				
305 K	18.58	59.2	36.4				
310 K	21.42	59.2	36.3				
315 K	21.09.	59.2	36.0				
		60.5	40.4				
		64.5	43.7, 44.7				
		64.5	46.5				
		$\Delta H_{fus}/(kJ\ mol^{-1})$ = 18.91					

Empirical temperature dependence equations:

Wauchope & Getzen (1972): $R{\cdot}\ln x = -[H_{fus}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b{\cdot}(T/K)$ (1)

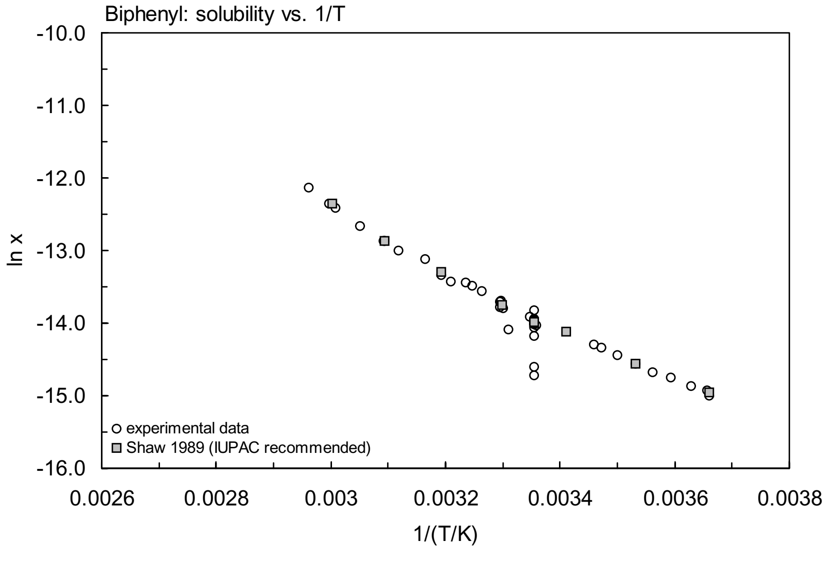


FIGURE 7.1.1.0.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for biphenyl.

TABLE 7.1.1.0.2
Reported vapor pressures of biphenyl at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)

$\log P = A - B/(C + t/°C)$ (2)

$\log P = A - B/(C + T/K)$ (3)

$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

$\log P = A - B/(T/K) - C/(T/K)^2$ (5)

$\ln P = A - B/(T/K)$ (1a)

$\ln P = A - B/(C + t/°C)$ (2a)

1.

Chipman & Peltier 1929		**Stull 1947**		**Bright 1951**		**Bradley & Cleasby 1953**	
isoteniscope-manometer		**summary of literature data**		**effusion**		**effusion**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
162.5	7933	70.6	133.3	Data presented in graph		15.05	0.416
172.3	10959	101.8	666.6	25	0.579	20.7	0.7786
177.7	12799	117.0	1333		(interpolated)	24.7	1.2252
183.5	15705	134.2	2666	eq. 1	P/mmHg	24.0	1.1825
191.6	19972	152.5	5333	A	10.38	24.1	1.184
198.75	24691	165.2	7999	B	3799	27.05	1.600
293.8	28504	180.7	13332	temp range 4.9–34.5°C		29.15	2.053
211.25	34677	204.2	26664			32.45	2.973
220.05	43756	229.4	53329	$\Delta H_{subl}/(kJ\ mol^{-1}) = 72.80$		35.05	3.866
229.8	56329	254.0	101325			37.9	5.160
238.2	68901					40.55	6.693
247.7	85580	mp/°C	69.5			23.05	1.027
253.7	98019					36.5	1.533
255.2	101178					31.25	2.546
						35.9	4.133
bp/°C	266.25						
$\Delta H_V/(kJ\ mol^{-1}) = 44.99$						eq. 1	P/mmHg
	at bp					A	11.282
						B	4262
eq. 5	P/mmHg					temp range 15–41°C	
A	7.0220						
B	1723						
C	245700						
temp range 162–322°C							

TABLE 7.1.1.0.2 *(Continued)*

2.

Radchenko& K. 1974		**Nasir et al. 1980**		**Burkhard et al. 1984**		**Cunningham 1930**	
Knudsen effusion		**pressure transducer**		**gas saturation-GC**		**in Boublik et al. 1984**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
24.9	1.433	123.0	2040	5.2	0.106	69.20	104
31.75	2.976	143.81	4773	14.9	0.361	93.3	413
33.7	3.734	164.69	9962	24.7	1.15	148.7	4833
35.5	4.538	181.28	16447			160.0	7239
37.6	5.726	200.87	28599	eq. 1	P/Pa	171.1	10548
39.57	6.913	223.66	51518	A	14.840	182.2	15031
41.52	8.26	245.65	86254	B	4402.1	193.3	21098
43.48	10.26	257.91	111343			204.4	28958
45.45	12.35	274.09	154493			215.6	39093
47.4	15.49	296.14	235345			226.7	51986
50.0	19.46	315.19	329300			237.8	68051
		327.55	400175			248.9	88252
eq. 1	P/mmHg					255.3	101353
A	12.6789	data fitted to				260.0	112384
B	4367.436	Chebyshev polynomial				271.2	142032
for temp range 24.9–50°C							
						eq. 2	P/kPa
						A	6.36895
Sharma & Palmer 1974						B	1997.558
gas saturation-GC						C	202.608
t/°C	**P/Pa**					bp/°C	255.208
53.05	16.0						
61.05	34.66						
71.95	92.0						
81.05	220.0						

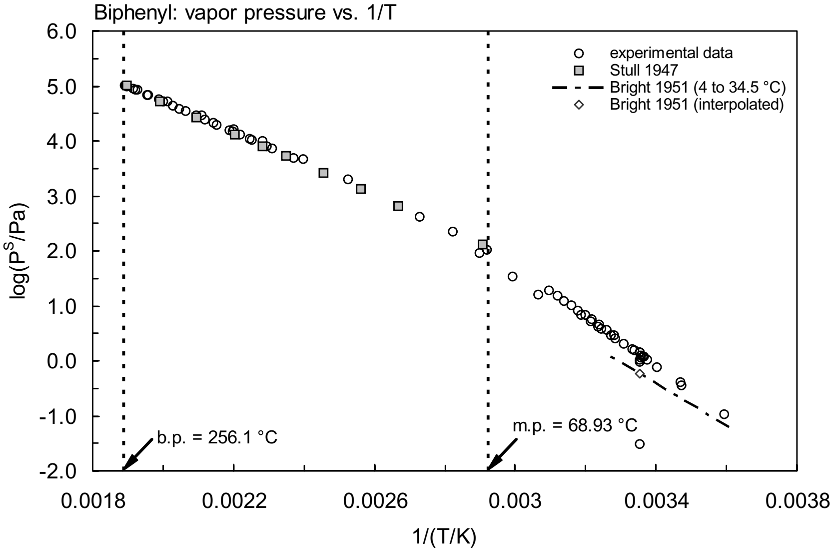
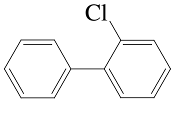


FIGURE 7.1.1.0.2 Logarithm of vapor pressure versus reciprocal temperature for biphenyl.

7.1.1.1 2-Chlorobiphenyl (PCB-1)



Common Name: 2-Chlorobiphenyl
Synonym: PCB-1, *o*-chlorobiphenyl, 2-chloro-1,1′-biphenyl
Chemical Name: 2-chlorobiphenyl
CAS Registry No: 2051-60-7
Molecular Formula: $C_{12}H_9Cl$
Molecular Weight: 188.652
Melting Point (°C):
34 (Beaven et al. 1961; Weast 1972–73, 1982–83; Lide 2003)
Boiling Point (°C):
274 (Weast 1972–73, 1082–83; Lide 2003)
Density (g/cm^3 at 20°C): 0.9837
Molar Volume (cm^3/mol):
205.5 (calculated-Le Bas method at normal boiling point)
172.9 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
57.8 (Geidarov et al. 1975)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
72.3 (Geidarov et al. 1975)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
14.52 (Geidarov et al. 1975)
15.3 (differential scanning calorimetry, Miller et al. 1984)
14.54 (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
47.66 (Geidarov et al. 1975)
50.21 (Miller et al. 1984)
Fugacity Ratio at 25°C, F (assuming ΔS_{fus} = 56 J/mol K), F: 0.816 (mp at 34°C)

Water Solubility (g/m^3 or mg/L at 25°C):
1.60 (Webb 1970)
0.90 (Hoover 1971)
5.90 (shake flask-GC/ECD, Wallnöfer et al. 1973)
4.13 (generator column-GC/ECD, Weil et al. 1974)
5.08 (supercooled liquid S_L, shake flask-GC/ECD, Chiou et al. 1983)
5.06 (generator column-GC/ECD, Miller et al. 1984,1985)
4.13, 4.74, 14.0, 4.13 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (89.3°C, summary of literature data, temp range 89.3–267.5°C, Stull 1947)
$\log(P/\text{mmHg}) = (8.306 \pm 0.087) - (3018 \pm 45)/(T/K)$, temp range: 410–510 K (static method-quartz manometer measurements, Geidarov et al. 1975)
1.84 (supercooled liquid P_L, extrapolated Antoine eq., Weast 1976–77)
1.12 (Neely 1981,1983)
0.605; 0.159; 0.367* (Knudsen effusion; torsion effusion; torsion-Knudsen effusion, extrapolated from exptl. derived Antoine eq., measured range 33–110°C, Ferro et al. 1983)

log (P_L/kPa) = – 3893/(T/K) + 9.99; temp range: 33–77°C (Knudsen effusion data, Ferro et al. 1983)
log (P_L/kPa) = – 4406/(T/K) + 10.98; temp range: 64–110°C (torsion effusion data, liquid, Ferro et al. 1983)
log (P_L/kPa) = – (4149 ± 230)/(T/K) + (10.48 ± 0.50); temp range: 33–110°C (torsion-Knudsen effusion data, Ferro et al. 1983)
1.096, 1.456 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
1.892, 2.56 (supercooled liquid P_L from P_{GC}, GC-RT correlation, different stationary phases, Bidleman 1984)
0.755 (GC-RI correlation, Burkhard et al. 1985a)
0.926 (GC-RI correlation, supercooled liquid P_L, Burkhard et al. 1985b)
2.20 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
1.096 (P_{GC} by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
log (P_L/Pa) = – 3366/(T/K) + 11.57 (GC-RT correlation, Falconer & Bidleman 1994)
0.27–2.70; 0.367–2.56 (literature P_S range; literature supercooled liquid P_L range, Delle Site 1997)
log (P/kPa) = 9.99 – 3893/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
28.9 (calculated-P/C, Burkhard et al. 1985b)
70.1 (calculated-P/C, Shiu & Mackay 1986)
74.6 (Dow Chemical, Neely 1982)
30.18 (calculated-QSPR, Dunnivant et al. 1992)
5.13, 8.32, 13.17, 20.43 ± 0.52, 29.3 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
K_{AW} = exp[– (42.7/kJ·mol^{-1})/ RT] + (0.104/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
22.0 (gas stripping-GC, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 43 ± 6 kJ/mol, ΔS_H = 0.10 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
4.54 (shake flask-GC, Tulp & Hutzinger 1978)
4.80 (Hansch & Leo 1979)
4.35 (HPLC-RT correlation, Veith et al. 1979)
4.10 (HPLC-RT correlation, McDuffie 1981)
4.59 ± 0.1; 4.56(shake flask-GC; RP-TLC-k′ correlation, Bruggeman et al. 1982)
3.75 (HPLC-RT correlation, Woodburn 1982)
4.51 (shake flask-GC, Chiou et al. 1983)
4.50 (generator column-GC, Miller et al. 1984,1985)
4.38 (generator column-HPLC, Woodburn et al. 1984)
3.90, 4.60 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.44 (HPLC-RP/MS correlation, Burkhard & Kuehl 1986)
4.38 (generator column-GC/ECD, Doucette & Andren 1987)
4.33, 4.39, 4.53, 4.43 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.92 (HPLC-RT correlation, Doucette & Andren 1988)
4.531 ± 0.029(shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
4.52 (recommended, Sangster 1989, 1993)
4.68 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated:
7.54, 6.65 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
6.04 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

3.50	(Woodburn silt loam soil, batch equilibrium isotherm-GC/ECD, Chiou et al. 1983)
4.35	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.47	(calculated, soil, Chou & Griffin 1986)
2.59	(Borden soil 0.29% OC, Hu et al. 1995)

Sorption Partition Coefficient, log K_{OM}:

3.23	(soil organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

k(calc) = 3.7×10^{-4} d^{-1} and with $t_{½}$ = 18 yr, calculated sunlight photolysis rate constant in surface water at 40°N in summer (Dulin et al. 1986)

k(calc) = 3.0 h^{-1} maximum summer photolysis rate, at midday under clear skies (Bunce et al. 1989)

$t_{½}$ = 31 d under sunlight in water (Mansour & Feicht 1994)

k = 0.081 min^{-1} at pH 3, k = 0.045 min^{-1} at pH 7 and k = 0.035 min^{-1} at pH 10 with half-lives of 9, 15 and 20 min, respectively, in aqueous solutions when irradiated by UVA-340 light tubes in the presence of 25 μg/mL of TiO_2;

k = (0.043–0.045) min^{-1} with $t_{½}$ = 15–16 min, k = (0.082–0.091) min^{-1} with $t_{½}$ = 8 min, and k = (0.21–0.29) min^{-1} with $t_{½}$ = 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively;

k = (0.043–0.044) min^{-1} with $t_{½}$ = 15–16 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2;

k = (0.030–0.055) min^{-1} with $t_{½}$ = 13–22 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.9 \pm 0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K with estimated atmospheric lifetime of ~8 d (relative rate method, Atkinson & Aschmann 1985)

$k_{OH} = 1.6 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to the C_6H_4Cl ring (ring B), $k_{OH} = 1.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to ring A, and $k_{OH} = 2.8 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)

k_{OH}(calc) = $(2.8 - 5.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = $(3.1 - 4.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)

$k_{OH} = 2.82 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (Atkinson 1989)

k_{OH}(exptl) = $(2.8 - 5.3) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = $(3.2 - 4.6) \times 10^{-12}$ cm^3 $molecule^{-1} \cdot s^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{½}$ = 100 h biodegradation by bacteria (Wong & Kaiser 1975);

within 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

k = 63 yr^{-1} microbial degradation pseudo first-order rate constant of in the water column and k = 630 yr^{-1} in the sediment (Wong & Kaiser 1975; quoted, Neely 1981);

k = 4.1 nmol L^{-1} d^{-1} biodegradation rate in water from Port Valdez with an initial concn of 1.5 μmol/L (data of Aug. 1977, Reichardt et al. 1981) and k = 1.2 nmol L^{-1} d^{-1} with initial concn of 4.5 μmol/L (data of Aug. 1978, Reichardt et al. 1981); and $t_{½}$ = 2–3.5 d, an initial concn of 1–100 μg/L by river dieaway test (Bailey et al. 1983)

k = 1.10 μg mL^{-1} d^{-1}, the degradation rate at 30 μg mL^{-1}, under culture conditions include river water as supportive medium and mixed bacterial cultures obtained from river sediments (Kong & Sayler 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of ~8 d due to reaction with the OH radical for a 24-h average OH radical concn of 5×10^5 cm^{-3} (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radical for mono-chlorobiphenyls (Atkinson 1987);

photolysis $t_{½}$ ~10–25 h for noontime summer sunshine, or more realistically, several days (Bunce et. 1989);

tropospheric lifetime of 3 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);

tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 1.4 d in Lake Michigan (Neely 1983);

photolysis $t_{½}$ = 18 yr in surface water at 40° L in summer (Dulin et al. 1986);

photolysis $t_{½}$ = 31 d under sunlight (Mansour & Feicht 1994);

half-lives in aqueous solutions with initial concn of 265 ng/mL, $t_{½}$ = 9 min at pH 3, $t_{½}$ = 15 min at pH 7 and $t_{½}$ = 20 min at pH 10 when irradiated by UVA-340 light tubes (simulated sun light) in the presence of 25 μg/mL TiO_2, half-lives of 15–16 min, 8 min and 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; half-lives of 15–16 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2; $t_{½}$ = 13–22 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 7.1.1.1.1

Reported vapor pressures of 2-chlorobiphenyl (PCB-1) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)

$\log (P/mmHg) = A - B/(C + t/°C)$ (2)

$\log (P/Pa) = A - B/(C + T/K)$ (3)

$\log (P/mmHg) = A - B/(T/K) - C \cdot \log (T/K)$ (4)

$\ln P = A - B/(T/K)$ (1a)

$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		**Geidarov et al. 1975**		**Ferro et al. 1983**			
compiled literature data		**static-quartz manometer**		**torsion effusion**		**Knudsen**	**average**
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**P/Pa**	**P/Pa**
				cell C			
89.3	133.3	exptl data presented as eq. 1		50	10.3	17.3	13.8
109.8	666.7	eq 1	P/mmHg	54	10.9	19.2	10.0
134.7	1333	A	8.306	59	16.2	24.8	20.5
151.2	2666	B	3018	63	25.6	36.9	32.2
169.9	5333	range: 137–267°C		cell C			
182.1	7999			50	8.1	12.8	10.4
197.0	13333	mp/°C	31.61	59	15.8	22.9	20.6
219.6	26664	bp/°C	24	69	34.1	51.1	46.1
243.8	53329			73	44.3	65.5	59.0
267.5	101325	$\Delta H_V/(kJ\ mol^{-1})$ = 57.78		77	63.3	85.8	78.0
		$\Delta H_{fus}/(kJ\ mol^{-1})$ = 14.52		81	83.5	115	99.2

(*Continued*)

TABLE 7.1.1.1.1 (*Continued*)

Stull 1947		**Geidarov et al. 1975**		**Ferro et al. 1983**			
compiled literature data		**static-quartz manometer**		**torsion effusion**		**Knudsen**	**average**
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**P/Pa**	**P/Pa**
mp/°C	34.0	ΔS_{fus}/(J mol^{-1}K^{-1}) = 47.66		86	120	163	142
		ΔH_{subl}/(kJ mol^{-1}) = 72.30		cell B			
				28	0.762	1.50	1.13
				33	1.52	2.36	1.93
				37	2.30	3.42	2.85
				40	3.05	4.13	3.59
				46	3.81	5.17	4.50
				50	4.57	6.10	5.34
				54	6.10	9.69	7.90
				eq. 1	P/mmHg	P/mmHg	P/mmHg
				A	10.98	9.99	10.48
				B	4406	3898	4149
				temp range: 64–110°C		33–86°C	
				ΔH_V/(kJ mol^{-1}) = 79.4			

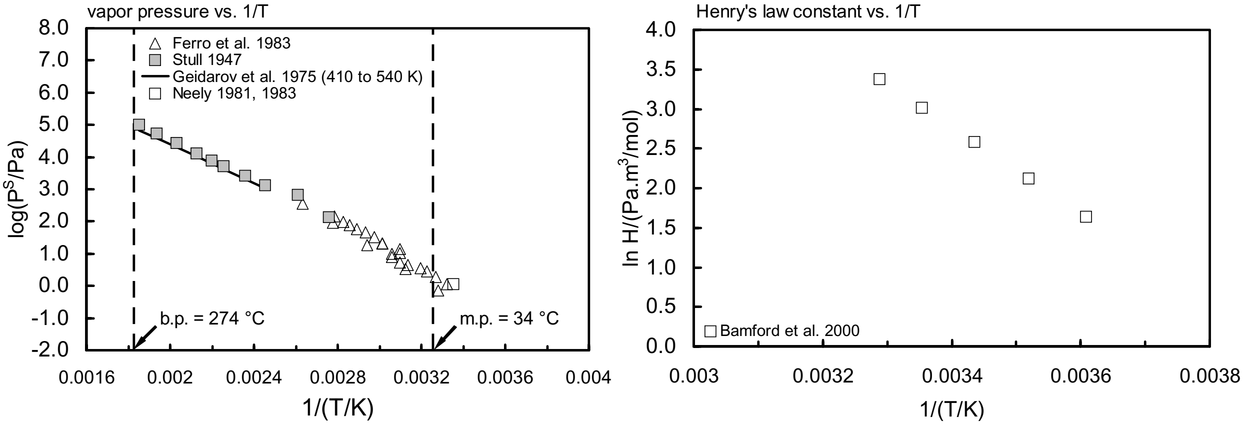
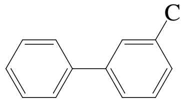


FIGURE 7.1.1.1.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for 2-chlorobiphenyl (PCB-1).

7.1.1.2 3-Chlorobiphenyl (PCB-2)



Common Name: 3-Chlorobiphenyl
Synonym: PCB-2, *m*-chlorobiphenyl, 3-chloro-1,1′-biphenyl
Chemical Name: 3-chlorobiphenyl
CAS Registry No: 2051-61-8
Molecular Formula: $C_{12}H_9Cl$
Molecular Weight: 188.652
Melting Point (°C):
16 (Weast 1972–73, 1982–83; Lide 2003)
Boiling Point (°C):
284.5 (Lide 2003)
Density (g/cm^3 at 20°C): 0.9837
Molar Volume (cm^3/mol):
205.5 (calculated-Le Bas method at normal boiling point)
172.9 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
15.31 (Miller et al. 1984)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0 (mp at 16°C)

Water Solubility (g/m^3 or mg/L at 25°C):
3.50 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
1.30 (generator column-GC/ECD, Weil et al. 1974)
0.56, 0.82, 0.88, 0.86 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.63 (generator column-HPLC/UV, Billington et al. 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.723 (extrapolated P_L, Antoine eq., Weast 1972–73)
0.711; 4.01; 0.362* (Knudsen effusion; torsion effusion; torsion-Knudsen effusion, extrapolated from exptl. derived Antoine eq., measured range 37–129°C, Ferro et al. 1983)
$\log (P_L/kPa) = -3458/(T/K) + 8.45$; temp range: 37–86°C (Knudsen effusion data, liquid, Ferro et al. 1983)
$\log (P_L/kPa) = -3371/(T/K) + 8.91$; temp range: 68–129°C (torsion effusion data, liquid, Ferro et al. 1983)
$\log (P_L/kPa) = -(3614 \pm 188)/(T/K) + (8.68 \pm 0.47)$; temp range: 37–129°C (torsion-Knudsen effusion data, Ferro et al. 1983)
0.98, 1.01 (supercooled P_L, GC-RT correlation with different stationary phases, Bidleman 1984)
0.366 (GC-RI correlation, Burkhard et al. 1985a)
0.362 (liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.997 (liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -3476/(T/K) + 11.65$ liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.220–1.01 (quoted lit. range, Delle Site 1997)
$\log (P/Pa) = 11.64178 - 3514.98/(T/K)$ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C):
14.49 (calculated-P/C, Burkhard et al. 1985b)
75.55 (calculated-P/C, Shiu & Mackay 1986)
62.11 (Dow Chemical, Neely 1982)
27.78 (calculated-QSAR, Dunnivant et al. 1992)

20.3	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

4.54	(shake flask-GC/ECD, Tulp & Hutzinger 1978)
4.35	(HPLC-RT correlation, Veith et al. 1979)
4.80	(Hansch & Leo 1979)
4.71 ± 0.1	(shake flask-GC/ECD, Bruggeman et al. 1982)
4.72	(RP-TLC-retention time correlation, Bruggeman et al. 1982)
4.35	(HPLC-RT correlation, Woodburn 1982)
4.58	(generator column-HPLC, Woodburn et al. 1984)
3.75	(HPLC-RT correlation, Woodburn et al. 1984)
4.60	(RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.60	(selected, Shiu & Mackay 1986)
4.58	(generator column.-GC/ECD, Doucette & Andren 1987)
4.65	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
4.58	(recommended, Sangster 1989, 1993)
4.72	(HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.58	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

7.86, 6.99	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
6.88	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

4.42	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.62	(calculated-S, soil, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

$t_{½}$ = 45 d under sunlight in water (Mansour & Feicht 1994)

k(calc) = 0.5 h^{-1}, maximum summer photolysis rate, at midday under clear skies (Bunce et al. 1989)

k = (0.036–0.045) min^{-1} with $t_{½}$ = 15–19 min, k = (0.069–0.085) min^{-1} with $t_{½}$ = 8–10 min, and k = (0.18–0.23) min^{-1} with $t_{½}$ = 3–4 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively;

rate constant of k = (0.027–0.042) min^{-1} with $t_{½}$ = 16–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2;

k = (0.033–0.036) min^{-1} with $t_{½}$ = 19–21 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (5.4 \pm 0.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 ± 1 K, with an estimated atmospheric lifetime of ~4 d (relative rate method, Atkinson & Aschmann 1985)

$k_{OH} = 2.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to the C_6H_4Cl ring (ring B), $k_{OH} = 1.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to ring A, and $k_{OH} = 5.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)

k_{OH}(calc) = $(2.8 - 5.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = $(3.1 - 4.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)

$k_{OH} = 5.28 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (Atkinson 1989)

k_{OH}(exptl) = (2.8 – 5.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = (3.2 – 4.6) × 10^{-12} cm^3 $molecule^{-1} \cdot s^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegradation $t_{1/2}$ ≈ 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumara 1976; selected, Pal et al. 1980);

biodegradation rate k ~ 2.6 nmol L^{-1} d^{-1} with an initial concentration of 3.6 μmol L^{-1} in water from Port Valdez estimated to be (data of August 1977, Reichardt et al. 1981);

biodegradation $t_{1/2}$ ~ 3–4 d for 50% initial concentration of 1–100 μg L^{-1} by river dieaway test (Bailey et al. 1983);

degradation rate k = 1.6 μg mL^{-1} d^{-1} at 30 μg mL^{-1} under culture conditions include river water as supportive medium and mixed bacterial cultures obtained from river sediments (Kong & Sayler 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 0.29 d^{-1}, 0.13 d^{-1}, 0.11 d^{-1}, 0.11 d^{-1} (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of ~ 4 d due to reaction with the OH radical for a 24-h average OH radical concn of 5 × 10^5 cm^{-3} (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 5–11 based on the calculated rate constant of gas-phase reaction with OH radicals for mono-chlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 2 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);

tropospheric lifetime of 2.7–5.1 d based on both the experimentally determined and calculated rate constant for reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: photolysis $t_{1/2}$ = 45 d under sunlight in water (Mansour & Feicht 1994);

$t_{1/2}$ = 15–19 min, 8–10 min and 3–4 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{1/2}$ = 16–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2; $t_{1/2}$ = 19–21 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 7.1.1.2.1
Reported vapor pressures of 3-chlorobiphenyl (PCB-2) at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K) (1) ln P = A – B/(T/K) (1a)
log P = A – B/(C + t/°C) (2) ln P = A – B/(C + t/°C) (2a)
log P = A – B/(C + T/K) (3)
log P = A – B/(T/K) – C·log (T/K) (4)

Ferro et al. 1983			
torsion effusion		Knudsen	average
T/K	**P/Pa**	**P/Pa**	**P/Pa**
cell B			
310	1.52	2.43	1.97
313	2.29	3.62	2.96
319	3.05	4.12	3.58

(Continued)

TABLE 7.1.1.2.1 (*Continued*)
Reported vapor pressures of 3-chlorobiphenyl (PCB-2) at various temperatures and the coefficients for the vapor pressure equations

Ferro et al. 1983			
torsion effusion		Knudsen	average
T/K	P/Pa	P/Pa	P/Pa
323	3.81	6.23	5.02
327	8.33	8.53	6.93
332	8.38	12.9	10.6
336	11.4	18.0	14.7
341	14.5	22.5	15.4
346	19.8	30.0	24.9
350	28.2	43.2	35.7
cell C			
332	13.6	19.1	16.3
336	15.8	22.3	19.0
341	23.4	29.0	26.2
346	27.5	35.6	31.5
350	33.7	46.2	40.0
354	47.3	63.6	55.4
359	63.2	84.9	74.0
eq. 1	P/mmHg	P/mmHg	P/mmHg
	torsion	Knudsen	average
A	8.91	8.45	8.68
B	3771	3458	3614
range, K	341–402	310–359	

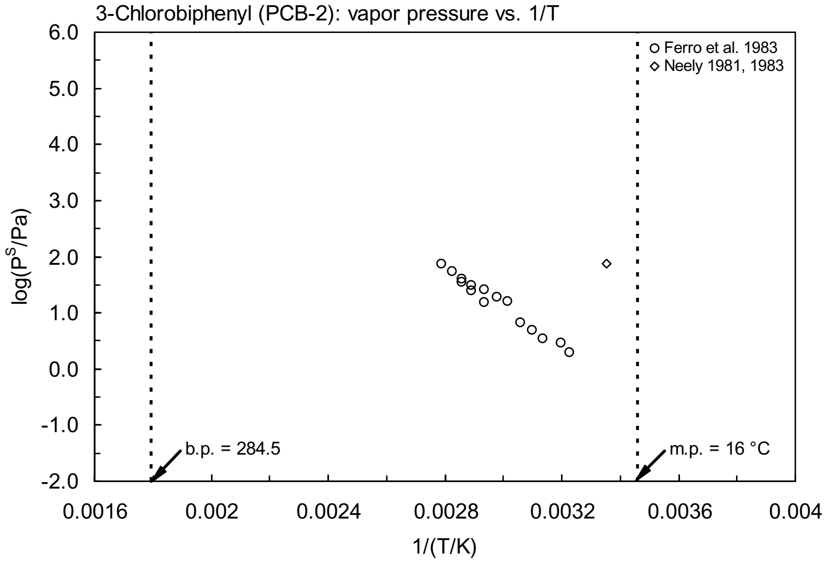
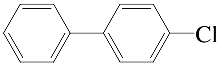


FIGURE 7.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 3-chlorobiphenyl (PCB-2).

7.1.1.3 4-Chlorobiphenyl (PCB-3)



Common Name: 4-Chlorobiphenyl
Synonym: PCB-3, *p*-chlorobiphenyl, 4-chloro-1,1′-biphenyl
Chemical Name: 4-chlorobiphenyl
CAS Registry No: 2051-62-9
Molecular Formula: $C_{12}H_9Cl$
Molecular Weight: 188.652
Melting Point (°C):
78.8 (Lide 2003)
Boiling Point (°C):
292.9 (Lide 2003)
Density (g/cm^3 at 20°C): 0.9837
Molar Volume (cm^3/mol):
205.5 (calculated-Le Bas method at normal boiling point)
172.9 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
65.94 (Geidarov et al. 1975)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
79.24 (Geidarov et al. 1975)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
13.32 (Geidarov et al. 1975; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.297 (mp at 78.8°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.0 (Webb 1970)
0.40 (Hoover, 1971)
1.19 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.90 (generator column-GC/ECD, Weil et al. 1974)
1.65 (Branson 1977)
0.0151 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
1.478* (generator column-GC/ECD, measured range 4–32°C, Stolzenburg & Andren 1983)
$\ln x = -3428/(T/K) - 4.2786$, ΔH_{ss} = 28.5 kJ/mol (regression eq. given by Dickhut et al. 1986, based on exptl data of Stolzenburg & Andren 1983)
$\log x = -1486/(T/K) - 1.850$; ΔH_{ss} = 28.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Stolzenburg & Andren 1983); or
$S/(mol/L) = 2.94 \times 10^{-8} \exp(0.041 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Stolzenburg & Andren 1983)
1.20 (selected, Shiu & Mackay 1986)
1.30, 1.38 (generator column-HPLC/UV, Billington et al. 1988)
0.82, 0.88, 0.84, 0.95 (RP- HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.207 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.81 (shake flask-LSC, [^{14}C] 4-monoCB, Eadie et al. 1990)
1.34 (shake flask-GC/ECD, Li et al. 1992; Li & Andren 1994)
1.32 (shake flask-GC/ECD, Li & Doucette 1993)
1.37* ± 0.042 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
$\ln x = -5.9137 - 2926.22/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
3.23, 3.81 (supercooled liquid: LDV literature-derived value, FAV final-adjusted value, Li et al. 2003)

log S_L/(mol m^{-3}) = – 631/(T/K) + 0.35 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log S_L/(mol m^{-3}) = – 963/(T/K) + 1.53 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (96.4°C, summary of literature data, temp range 96.4–292.9°C, Stull 1947)
1.41 (supercooled liq. P_L, Weast 1972–1973)
log (P/mmHg) = (9.037 ± 0.635) – (3445 ± 18)/(T/K), temp range: 452–536 K (static method-quartz manometer measurements, Geidarov et al. 1975)
0.61 (Neely 1981,1983)
0.339*; 0.253 (P_S- Knudsen effusion; P_L-torsion effusion, extrapolated from exptl. derived from Antoine eq., Ferro et al. 1983)
log (P_S/kPa) = – (3849 ± 200)/(T/K) + (9.44 ± 0.63); temp range 33–73°C (Knudsen effusion data, solid, Ferro et al. 1983)
log (P_L/kPa) = – (3541 ± 250)/(T/K) + (8.28 ± 0.55); temp range 75–136°C (torsion effusion data, liquid, Ferro et al. 1983)
1.41 (supercooled liquid P_L, converted from literature P_S, Bidleman 1984)
0.951, 0.567 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.92, 0.942 (supercooled liquid P_L from P_{GC}, GC-RT correlation, different GC columns, Bidleman 1984)
0.175* (gas saturation-GC, measured range 5.2–24.9°C, Burkhard et al. 1984; Burkhard et al. 1985a)
log (P_S/Pa) = – 4754.1/(T/K) + 15.188; temp range: 5.2–24.9°C (gas saturation-GC, Clapeyron eq. Burkhard et al. 1984)
0.0979 (GC-RI correlation, Burkhard et al. 1985a)
0.320 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.907 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
0.270, 0.90 (selected P_S, supercooled P_L, Shiu & Mackay 1986)
0.593 (P_{GC} by GC-RT correlation, Hinckley et al. 1990)
0.275 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 3488/(T/K) + 11.67 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
0.0677* (20°C, as saturation-GC/ECD, Wania et al. 1994)
log (P_S/Pa) = – 4493/(T/K) + 14.15; temp range: – 20 to 30°C (gas saturation-GC, Wania et al. 1994)
0.087–0.339; 0.253–0.942 (quoted literature P_S range; literature P_L range, Delle Site 1997)
log P/kPa = 15.188 – 4751.1/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.468, 0.479 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = – 3737/(T/K) + 12.21 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log P_L/Pa = – 3627/(T/K) + 11.84 (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

58.06 (batch stripping, Atlas et al. 1982; Dow Chemical, Neely 1982))
42.56 (calculated-P/C, Shiu & Mackay 1986)
34.14 (batch stripping-GC, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
24.39 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
23.30 (wetted-wall column-GC, Brunner et al. 1990)
5.84 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
18.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 56 ± 27 kJ/mol, ΔS_H = 0.15 ± 0.10 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
36.3, 23.44 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2664/(T/K) + 10.31 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

4.90 (Branson 1977)
4.26 (Sugiura et al. 1978)
4.80 (Hansch & Leo 1979)
4.61 ± 0.1 (shake flask-GC, Bruggeman et al. 1982)

4.69 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
4.34 (HPLC-RT correlation, Woodburn 1982)
4.49 (generator column-HPLC, Woodburn et al. 1984)
4.34 (HPLC-RT correlation, Woodburn et al. 1984)
4.40 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.49 (generator column-GC/ECD, Doucette & Andren 1987,1988)
4.55, 4.73, 4.64, 4.59 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.53, 4.27 (RP-HPLC-k′ correlation, different stationary phases, Sherbolm & Eganhouse 1988)
4.61 (recommended, Sangster 1989, 1993)
4.72 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.37 (generator column-HPLC, Li & Doucette 1993)
4.61 (recommended, Hansch et al. 1995)
4.49, 4.65 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.01* (generator column-GC; measured range – 10 to 30°C, Harner & Mackay 1995)
log $K_{OA} = -6.50 + 3962/(T/K)$; temp range –10 to 20°C, (generator column-GC, Harner & Mackay 1995)
7.01* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log $K_{OA} = -4.82 + 3470/(T/K)$; temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
7.86, 6.99; 6.99 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
7.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
6.80; 6.93 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
6.82, 6.78 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log $K_{OA} = 3520/(T/K) - 4.97$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

2.08 (killifish, Goto et al. 1978)
2.68 (NAS 1979)
2.77 (estimated, fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
2.67 (calculated-solubility, Kenaga 1980)
3.88 (fish, normalized, lipid basis, Tadokoro & Tomita 1987)
2.77, 4.07 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

3.52 (calculated, Kenaga 1980)
4.43 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.90 (soil, calculated-S, Chou & Griffin 1986)
4.71 (Great Lake suspended matter, phase partitioning-reversed phase chromatography by Sep Pak, Eadie et al. 1990)
4.70 (Green Bay suspended matter, reversed phase separation, Eadie et al. 1992)
3.49 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Sorption Partition Coefficient, log K_{OM}:

4.02 (Great Lakes DOC, reversed phase separation, Eadie et al. 1990)
4.61 (Green Bay DOC, reversed phase separation, Eadie et al. 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
$k = 2.3 \times 10^{-4}\ d^{-1}$ with $t_{1/2} = 8.2$ yr in surface water at 40°N in summer sunlight is (Dulin et al. 1986)
$t_{1/2} = 45$ d in water (Mansour & Feicht 1994)

k(calc) = 13.5 h^{-1}, maximum summer photolysis rate calculated under midday clear skies, experimental k(exptl) ~1.0×10^{-8} mol s^{-1}, irradiated with a low-pressure mercury lamp (Bunce et al. 1989)

k = (0.036–0.045) min^{-1} with $t_{½}$ = 15–19 min, k = (0.048–0.082) min^{-1} with $t_{½}$ = 8–14 min and k = (0.13–0.30) min^{-1} with $t_{½}$ = 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively;

k = (0.027–0.046) min^{-1} with $t_{½}$ = 15–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2;

k = (0.022–0.038) min^{-1} with $t_{½}$ = 18–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (3.9 \pm 0.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 ± 1 K, with an estimated atmospheric lifetime of ~6 d (relative rate method, Atkinson & Aschmann 1985)

$k_{OH} = 2.6 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to the C_6H_4Cl ring (ring B), $k_{OH} = 1.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to ring A, and $k_{OH} = 3.8 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)

k_{OH}(calc) = $(2.8 – 5.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = $(3.1 – 4.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)

$k_{OH} = 5.28 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (Atkinson 1989)

k_{OH}(exptl) = $(2.8 – 5.3) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = $(3.2 – 4.6) \times 10^{-12}$ cm^3 $molecule^{-1} \cdot s^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{½}$ = 175 h biodegradation by bacteria (Wong & Kaiser 1975; quoted, Pal et al. 1980);

within 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980)

k = 38 yr^{-1} in the water column, and k = 380 yr^{-1} in the sediment, pseudo first-order rate constant for microbial degradation (Wong & Kaiser 1975; quoted, Neely 1981)

k = 3.1 nmol L^{-1} d^{-1} with an initial concentration of 2.9 µmol/L, degradation rate in water from Port Valdez(data of Aug. 1977, Reichardt et al. 1981); $t_{½}$ = 2–5 d, time for 50% degradation of an initial concentration of 1–100 µg L^{-1} by river dieaway test (Bailey et al. 1983)

k = 2.0 µg mL^{-1} d^{-1} at 30 µg mL^{-1}, under culture conditions include river water as supportive medium and mixed bacteria cultures obtained from river sediments (Kong & Sayler 1983)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.01 d^{-1} with $t_{½}$ = 67 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of ~6 d due to reaction with the OH radical for a 24-h average OH radical concn of 5×10^5 cm^{-3} (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radical for mono-chlorobiphenyls (Atkinson 1987);

photolysis $t_{½}$ ~10–25 h for noontime summer sunshine, or more realistically, several days (Bunce et. 1989);

tropospheric lifetime of 3 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);

tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 4.9 d in Lake Michigan (Neely 1983);

photolysis $t_{½}$ = 8.2 yr in summer sunlight at 40°L in surface waters (Dulin et al. 1986);

photolysis $t_{1/2}$ = 45 d, sunlight days in water (Mansour & Feicht 1994)

$t_{1/2}$ = 15–19 min, 8–14 min and 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2 respectively; $t_{1/2}$ = 15–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{1/2}$ = 18–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 88 d for high-dose treatment, $t_{1/2}$ = 67 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.3.1
Reported aqueous solubilities and octanol-air partition coefficients of 4-chlorobiphenyl (PCB-3) at various temperatures

Aqueous solubility				log K_{OA}			
Stolzenburg & Andren 1983		Shiu et al. 1997		Harner & Mackay 1995		Harner & Bidleman 1996	
generator column-GC/ECD		generator column-GC/ECD		generator column-GC		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	log K_{OA}	t/°C	log K_{OA}
4	0.661	5	0.822	–10	8.65	–10	8.34
20	1.206	15	1.07	0	8	0	7.91
25	1.478	25	1.37	10	7.48	10	7.43
32	2.128	35	2.17	20	7.01	20	7.01
		45	3.04	25	6.76	30	6.62
ΔH_{sol}/(kJ mol^{-1}) = 28.5		ΔH_{sol}/(kJ mol^{-1}) = 24.5		ΔH_{OA}/(kJ mol^{-1}) = 75.9		ΔH_{OA}/(kJ mol^{-1}) = 75.86	
for 5–45°C		for 5–45°C					
				log K_{OA} = A + B/T		log K_{OA} = A + B/T	
				A	–6.52	A	–4.82
				B	3962.2	B	3470

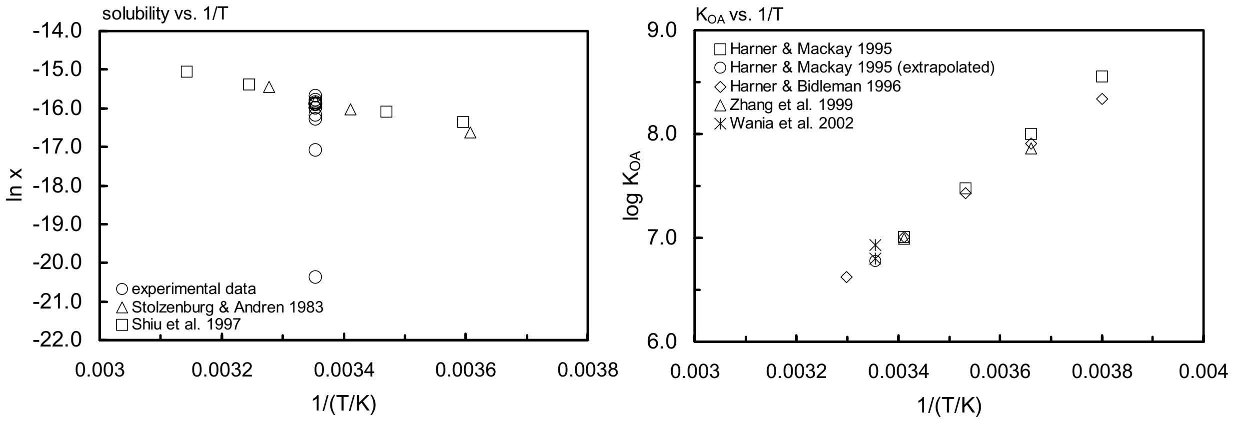


FIGURE 7.1.1.3.1 Logarithm of mole fraction solubility and K_{OA} versus reciprocal temperature for 4-chlorobiphenyl (PCB-3).

TABLE 7.1.1.3.2
Reported vapor pressures of 4-chlorobiphenyl (PCB-3) at various temperatures and the coefficients for the vapor pressure equations:

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log(T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

1.

Stull 1947		**Geidarov et al. 1975**		**Ferro et al. 1983**			
compiled literature data		**static-quartz manometer**		**torsion-effusion**		**Knudsen**	**average**
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**P/Pa**	**P/Pa**
				cell B			
96.4	133.3	data presented in graph and		33	0.762	0.697	0.729
129.8	666.7			37	1.52	0.902	1.21
146.0	1333	eq 1	P/mmHg	50	3.05	3.57	3.31
164.0	2666	A	9.037	54	3.81	4.90	4.38
183.8	5333	B	3445	59	6.10	7.41	6.75
196.0	7999	range: 179–263°C		63	9.14	10.4	9.77
212.6	13333			73	21.3	18.3	19.8
237.8	26664	mp/°C	74.75	cell B			
284.5	53329	bp/°C	287	35	0.762	0.917	0.840
292.9	101325			41	1.62	1.41	1.47
		$\Delta H_V/(kJ\ mol^{-1}) = 65.94$		44	2.29	1.72	2.00
mp/°C	75.5	$\Delta H_{fus}/(kJ\ mol^{-1}) = 13.32$		50	3.05	2.85	2.95
		$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1}) = 38.3$		52	3.81	4.44	4.12
		$\Delta H_{subl}/(kJ\ mol^{-1}) = 79.24$		57	5.33	6.04	5.69
				61	7.62	8.43	8.03
				62	8.38	10.9	9.66
				65	10.7	10.8	10.8
				67	12.9	11.9	12.4
				68	13.7	12.9	13.3
				69	15.2	13.9	14.6
				73	21.1	18.6	15.3
				eq. 1	P/mmHg	P/mmHg	
				A	8.28	9.44	
				B	3541	3849	
				range, °C	75–136(liq.)	33–73(solid)	
				$\Delta H_V/(kJ\ mol^{-1}) = 67.8$			

TABLE 7.1.1.3.2 *(Continued)*

2.

Burkhard et al. 1984		**Wania et al. 1994**	
gas saturation-GC		**gas saturation-GC**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**
4.2	0.0111	–20	2.446×10^{-4}
15.0	0.0493	–10	1.297×10^{-3}
24.9	0.172	0	4.889×10^{-3}
25.0	0.175	10	1.883×10^{-2}
		20	6.771×10^{-2}
		30	0.2233
eq. 1	P/Pa		
A	15.188	eq. 1	P/Pa
B	4754.1	A	14.15
range: 4.2–25°C		B	4493
		temp range –20 to30°C	
		$\Delta H_{subl}/(\text{kJ mol}^{-1}) = 86.0$	

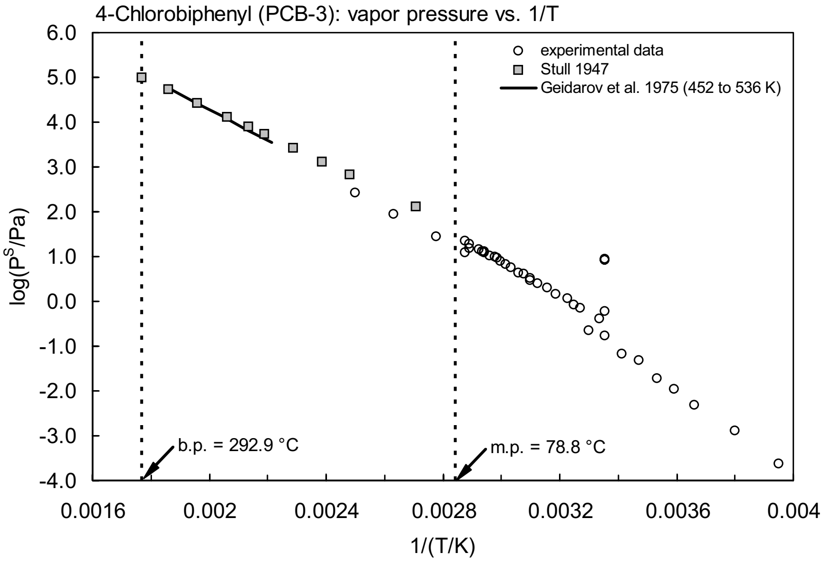
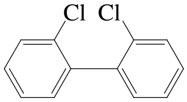


FIGURE 7.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-chlorobiphenyl (PCB-3).

7.1.1.4 2,2′-Dichlorobiphenyl (PCB-4)



Common Name: 2,2′-Dichlorobiphenyl
Synonym: PCB-4, 2,2-dichloro-1,1′-biphenyl
Chemical Name: 2,2′-dichlorobiphenyl
CAS Registry No: 13029-08-8
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
  60.5 (Hutzinger et al. 1974)
Boiling Point (°C):
  312 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
  226.4 (calculated-Le Bas method at normal boiling point)
  185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.448 (mp at 60.5°C)
  0.442 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
  1.0 (Webb 1970)
  0.90 (Hoover 1971)
  1.50 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
  0.79 (generator column-GC/ECD, Weil et al. 1974)
  0.0212 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
  1.86 (20°C, supercooled liquid, shake flask-GC/ECD, Chiou et al. 1982,1983; Chiou 1985)
  1.124 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  0.511, 0.322, 0.362, 0.511 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  1.207 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.133 (Knudsen-effusion technique, extrapolated from 37–54.92°C, Smith et al. 1964)
  0.36 (quoted, Neely 1981)
  0.82 (P_L calculated from P_S using F, Neely 1981)
  0.189 (GC-RI correlation, Burkhard et al. 1985a)
  0.424 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985a)
  0.326, 0.335 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.134 (extrapolated-Antoine eq., solid, Stephenson & Malanowski 1987)
  $\log (P_S/kPa) = -5019/(T/K) + 12.962$; temp range 37–55°C (Antoine eq., Stephenson & Malanowski 1987)
  0.152 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  0.275, 0.363 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
  $\log (P_L/Pa) = -3462/T + 11.73$ (supercooled liquid P_L, GC-RT, Falconer & Bidleman 1994)
  0.0603–0.315; 0.280–0.424 (quoted literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
  30.2 (20°C, calculated-P/C, Murphy et al. 1987)
  34.14 (batch stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
  23.3 (wetted-wall column-GC, Brunner et al. 1990)

8.02 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
23.0(from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 50 \pm 25$ kJ/mol, $\Delta S_H = 0.13 \pm 0.09$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.04 (HPLC-RT correlation, Sugiura et al. 1978)
5.70 (HPLC-RT correlation, Sugiura et al. 1979)
5.51 (Hansch & Leo 1979)
4.00 (HPLC-k′ correlation, McDuffie 1981)
5.00 ± 0.1 (shake flask-GC, Bruggeman et al. 1982)
3.02 (RP-TLC-retention correlation, Bruggeman et al. 1982)
3.55 (HPLC-RT correlation, Woodburn 1982)
4.80 (shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
4.90; 3.55 (generator column-GC/ECD; HPLC-RT correlation, Woodburn et al. 1984)
3.63; 4.89 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
4.90 (generator column-GC/ECD, Doucette & Andren 1987,1988)
4.25, 4.86, 4.65, 4.94(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.965 ± 0.013(slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.09 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.73 (recommended, Sangster 1993)
4.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:
7.18; 6.56 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log $K_{OA} = -4.84 + 3590/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
7.66, 6.86 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
6.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
2.04 (killifish, Goto et al. 1978)
3.72, 2.95, 3.60, 3.26 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
– 1.40, – 1.30, – 1.35 (adipose tissue of male, female Albino rats, rodents, Geyer et al. 1980)
2.05, 2.45 (fish: flowing water, microcosm condition Garten & Trabalka 1983)
3.43, 2.90 (algae, calculated, Geyer et al. 1984)
3.43, 3.38, 3.80(algae, fish, activated sludge, Freitag et al. 1984,1985)
3.85 (fish, normalized, lipid basis, Tadokoro & Tomita 1987)
3.38; 3.413, 3.715(quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
3.68 (Woodburn silt loam soil, soil organic matter, sorption isotherm-GC, Chiou et al. 1983)
4.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.84 (soil, calculated-S, Chou & Griffin 1986)
3.92 (soil, calculated-MCI, Sabljic et al. 1995)
3.96; 3.92 (soil, calculated-Characteristic Root Index CRI; quoted lit., Saçan & Balcioğlu 1996)
4.30 (soil, calculated-K_{OW}, Girvin & Scott 1997)
4.90; 3.90 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Sorption Partition Coefficient, log K_{OM} at 25°C or as indicated:
3.68 (20°C, Wood burn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
3.68, 4.18 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated $t_{½}$ ~ 3.1 h of evaporation with an initial concentration of 0.1 ppm from 4.5 cm depth of water solution in a glass dish at 24°C is 3.1 h and $t_{½}$ = 0.4 h with stirring of the solution; the experimental $t_{½}$ = 3.9 h and 0.9 h of evaporation under same condition with stirring of the solution (Chiou et al. 1979).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.4×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

k_{OH}(calc) = $(1.4 - 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH} = $(2.0 \pm 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{O3} < 2.0×10^{-20} cm^3 $molecule^{-1}$ s^{-1} at 297 ± 2 K (relative rate method, Kwok et al. 1995)

tropospheric lifetime τ(calc) = 3.4–7.2 d, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 - 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 - 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: Biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 but small residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

microbial degradation with pseudo first-order k = 0.65 yr^{-1} in the water column and k = 6.5 yr^{-1} in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.027 d^{-1} (10°C, sandworm, Goerke & Erst 1977; quoted, Waid 1986)

k_1 = 0.29 d^{-1}, 0.13 d^{-1}, 0.11 d^{-1}, 0.11 d^{-1} (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

k_2 = 0.017 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

k_1 = 122 d^{-1}; k_2 = 0.014 d^{-1} (rainbow trout, calculated, Gobas & Mackay 1987)

k_2 = 0.004 d^{-1} with $t_{½}$ = 183 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 93 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 34.5 d in Lake Michigan (Neely 1983)

Groundwater:

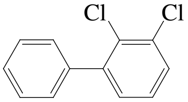
Sediment:

Soil:

Biota: $t_{½}$ = 40 d in rainbow trout, and $t_{½}$ = 20 d in its muscle (Niimi & Oliver 1983).

Depuration $t_{½}$ = 183 d for high-dose treatment, $t_{½}$ = 93 d for high-dose + enzyme treatment (juvenile rainbow trout, Buckman et al. 2004)

7.1.1.5 2,3-Dichlorobiphenyl (PCB-5)



Common Name: 2,3-Dichlorobiphenyl
Synonym: PCB-5, 2,3-dichloro-1,1′-biphenyl
Chemical Name: 2,3-dichlorobiphenyl
CAS Registry No: 16605-91-7
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C): 28.0
  27.8–28.2 (Erickson 1985)
Boiling Point (°C):
  172 (at 4000 Pa, Erickson 1986)
Density (g/cm^3):
Molar Volume (cm^3/mol):
  226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.934 (mp at 28°C)

Water Solubility (g/m^3 or mg/L at 25°C):
  1.70 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
  1.31, 1.23, 0.756, 0.829 (quoted lit.; RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  1.00, 0.658 (quoted average of Brodsky & Ballschmiter 1988, calculated-MCI χ, Patil 1991)
  1.36 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.147, 0.144, 0.114(calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
  0.151 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985b)
  0.162 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
  $\log (P_L/Pa) = -3769/(T/K) + 11.81$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
  19.56 (calculated-P/C, Burkhard et al. 1985b)
  28.57 (calculated-MCI χ, Sabljic & Güsten 1989)
  23.30 (wetted-wall column-GC, Brunner et al. 1990)
  24.19 (calculated-QSPR, Dunnivant et al. 1992)
  8.97 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  24.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 48 \pm 24$ kJ/mol, $\Delta S_H = 0.12 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  5.20 (RP-TLC-RT correlation, Bruggeman et al. 1982)
  4.82, 4.92, 5.17, 5.05 (RP-PLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  4.99 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
  7.40; 6.98 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
  $\log K_{OA} = -5.41 + 3820/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)

8.55, 7.59 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:
3.08 (oyster, Vreeland 1974)
3.45–4.11 mean 4.11 (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
4.41; 4.11 (rainbow trout, 15°C, kinetic BCF k_1/k_2, steady-state BCF C_F/C_W, Oliver & Niimi 1985)
4.11, 5.25; 3.388, 3.895 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
3.08, 5.33 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.11, 5.20 (rainbow trout: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
4.76 (suspended particulate matter, Burkhard 1984)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis: rate constant k = (0.031–0.036) min^{-1} with $t_{½}$ = 19–23 min, k = (0.054–0.067) min^{-1} with $t_{½}$ = 10–13 min and k = (0.22–0.25) min^{-1} with $t_{½}$ = 3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA–340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; k = (0.022–0.028) min^{-1} with $t_{½}$ = 25–32 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2; k = (0.022–0.024) min^{-1} with $t_{½}$ = 29–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)
k_{OH-}(aq.) = 7.9×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
tropospheric lifetime τ(calc) = 3.4–7.2 d, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.011 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 300 d^{-1}; k_2 = 0.011 d^{-1} (rainbow trout, Oliver & Niimi 1985)
log $1/k_2$ = 2.0, 2.2 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).
Surface water: $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

$t_{½}$ = 19–23 min, 10–13 min and 3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{½}$ = 16–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2; $t_{½}$ = 29–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

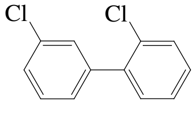
Groundwater:

Sediment:

Soil:

Biota: $t_{½}$ = 61 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{½}$ = 26 d in its muscle (Niimi & Oliver 1983).

7.1.1.6 2,3′-Dichlorobiphenyl (PCB-6)



Common Name: 2,3′-Dichlorobiphenyl
Synonym: PCB-6
Chemical Name: 2,3′-dichlorobiphenyl
CAS Registry No: 25569-80-6
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
36 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.605 (supercooled liquid S_L, Burkhard et al. 1985a)
0.580 (20°C, supercooled liquid S_L, Murphy et al. 1987)
1.226 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.928 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.165 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.157, 0.169, 0.0754 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.173, 1.208 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0799 (20°C, supercooled liquid, Murphy et al. 1987)
0.141, 0.178 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -3769/(T/\text{K}) + 11.88$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
27.76 (calculated-P/C, Burkhard et al. 1985a)
30.0 (20°C, calculated-P/C, Murphy et al. 1987)
39.42 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
25.33 (wetted-wall column-GC, Brunner et al. 1990)
33.09 (calculated-QSPR, Dunnivant et al. 1992)
4.016, 11.74 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
9.14 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
24.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 24$ kJ/mol, $\Delta S_H = 0.12 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (calculated-TSA, Burkhard 1984)
5.02 (quoted and selected, Brownwell & Farrington 1985)
4.84 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

5.06 (calculated-TSA, Hawker & Connell 1988a)
5.02 (recommended, Hansch et al. 1995)
5.044 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
8.51; 7.55 (0; 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

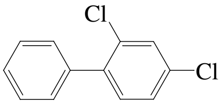
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
4.83 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis: $k = (0.018–0.052)\ \text{min}^{-1}$ with $t_{1/2}$ = 13–38 min, irradiated by sunlight in the presence of 100 µg/mL TiO_2 of diCBs in St. Lawrence River water containing 3 ng/mL of total PCB (Huang et al. 1996)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(\text{calc}) = 2.1 \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d, based on $k_{OH}(\text{calc.}) = (1.4 – 2.9) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ for dichlorobiphenyl at room temp. (Atkinson 1987)
$k_{OH\text{-}}(\text{aq.}) = 8.0 \times 10^9\ \text{dm}^3\ \text{mol}^{-1}\ \text{s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
tropospheric lifetime τ(calc) = 3.4–7.2 d, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0 – 4.2) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$, and the calculated $k_{OH}(\text{calc}) = (1.4 – 3.1) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.012\ \text{d}^{-1}$ with $t_{1/2}$ = 56 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.013\ \text{d}^{-1}$ with $t_{1/2}$ = 53 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical (Kwok et al. 1995).
Surface water: half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);
$t_{1/2}$ = 13–38 min for dichlorobiphenyl in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{1/2}$ = 56 d for high-dose treatment, $t_{1/2}$ = 53 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.7 2,4-Dichlorobiphenyl (PCB-7)



Common Name: 2,4-Dichlorobiphenyl
Synonym: PCB-7, 2,4-dichloro-1,1′-biphenyl
Chemical Name: 2,4-dichlorobiphenyl
CAS Registry No: 33284-50-3
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
  24.1–24.4 (Dickerman & Weiss 1957; Weingarten 1961; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
  226.4 (calculated-Le Bas method at normal boiling point)
  185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  1.0 (calculated, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  1.40 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
  0.637 (shake flask-GC/ECD, Haque & Schmedding 1975)
  1.13 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)
  0.587, 0.535, 0.689, 0.659 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  1.148 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C):
  0.184, 0.321 (supercooled liquid P_L, GC-RT correlation, different GC columns, Bidleman 1984)
  0.175 (supercooled liquid P_L, Burkhard et al. 1984)
  0.179 (GC-RI correlation, Burkhard et al. 1985a)
  0.175 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  0.210, 0.216 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.170, 0.195 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)

Henry's Law Constant (Pa m^3/mol at 25°C):
  96.66 (gas stripping-GC, Atlas et al. 1982)
  35.26 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
  28.37 (wetted-wall column.-GC/ECD, Brunner et al. 1990)
  24.78 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
  11.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  28.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 43 \pm 22$ kJ/mol, $\Delta S_H = 0.11 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  5.15 (RP-TLC-RT correlation, Bruggeman et al. 1982)
  4.67 (HPLC-RT correlation, Rapaport & Eisenreich 1984)

5.09, 5.21, 5.20, 5.10 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.13 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.16 (recommended, Sangster 1993)
5.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
8.37, 7.39; 7.25(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
6.98 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
4.83 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half Lives, $t_{½}$:
Volatilization:
Photolysis: calculated sunlight $k < 2 \times 10^{-8}$ s^{-1} and 5.7×10^{-11} s^{-1}, with $t_{½} > 400$ d at 40°N latitude in winter (Dulin et al. 1986);
k = (0.30–0.036) min^{-1} with $t_{½}$ = 19–23 min, k = (0.054–0.067) min^{-1} with $t_{½}$ = 10–13 min and k = (0.13–0.21) min^{-1} with $t_{½}$ = 3–5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; rate constants k = (0.015–0.043) min^{-1} with $t_{½}$ = 36–29 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2; rate constants k = (0.018–0.022) min^{-1} with $t_{½}$ = 31–38 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 - 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)
$k_{OH\text{-}}$(aq.) = 7.1×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 - 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the k_{OH}(calc) = $(1.4 - 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation: biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 from lake sediments but small amount residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.004 d^{-1} with $t_{½}$ = 192 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.005 d^{-1} with $t_{½}$ = 149 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH· oxidation (Sedlak & Andren 1991);

$t_{1/2}$ = 19–23 min, 10–13 min and 3–5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2 respectively; $t_{1/2}$ = 36–29 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{1/2}$ = 31–38 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

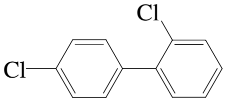
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 192 d for high-dose treatment, $t_{1/2}$ = 149 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.8 2,4′-Dichlorobiphenyl (PCB-8)



Common Name: 2,4′-Dichlorobiphenyl
Synonym: PCB-8, 2,4′-dichloro-1,1′-biphenyl
Chemical Name: 2,4′-dichlorobiphenyl
CAS Registry No: 34883-43-7
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
  46 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
  226.4 (calculated-Le Bas method at normal boiling point)
  185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.66 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  0.50 (Webb 1970; Hoover 1971)
  1.88 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
  0.637 (shake flask-GC, Haque & Schmedding 1975)
  0.620 (generator column-GC/ECD, Weil et al. 1974)
  0.139 (shake flask-GC/ECD from Aroclor 1242 mixture, Lee et al. 1979)
  1.17 (20°C, supercooled liquid P_L, shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985)
  0.974, 0.848, 0.643, 0.658 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  1.58, 1.45 (supercooled liquid S_L: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
  $\log S_L/(\text{mol m}^{-3}) = -1000/(T/K) + 1.17$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  0.0998 (GC-RI correlation, Burkhard et al. 1985a)
  0.147 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  0.157, 0.143 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  $\log (P/\text{mmHg}) = 9.74 - 3840/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
  0.129, 0.158 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
  $\log (P_L/\text{Pa}) = -3769/(T/K) + 11.84$ (GC-RT correlation, Falconer & Bidleman 1994)
  0.123, 0.148 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
  $\log P_L/\text{Pa} = -3818/(T/K) + 11.90$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
  $\log P_L/\text{Pa} = -3728/(T/K) + 11.68$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°Cor as indicated and reported temperature dependence equations):
  96.7 (gas stripping-GC, Atlas et al. 1982)
  23.30 (wetted wall column-GC/ECD, Brunner et al. 1990)
  35.67 ± 2.7 (gas stripping-GC/ECD; Girvin et al. 1997)
  6.01, 9.87, 15.85, 24.89* ± 0.29, 36.07 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
  $\ln K_{AW} = 13.2307 - 5304.31/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
  $K_{AW} = \exp[-(44.1/\text{kJ·mol}^{-1})/RT] + (0.110/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 $\text{J·K}^{-1}\text{·mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)

25.7 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 44 \pm 3$ kJ/mol, $\Delta S_H = 0.11 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
26.3, 22.9 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log H/(Pa m^3/mol) = – 2428/(T/K) + 9.56 (LDV linear regression of literature data, Li et al. 2003)
log H/(Pa m^3/mol) = – 2728/(T/K) + 10.51 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
5.51 (Hansch & Leo 1979)
4.48 (HPLC-RT correlation, Woodburn 1982)
5.10 (shake flask-GC, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
5.10 ± 0.4 (selected, Shiu & Mackay 1986)
5.14 (generator column-GC/ECD, Woodburn et al. 1984)
4.47; 5.10 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
5.14 (generator column-GC/ECD, Doucette & Andren 1987,1988)
4.93, 5.05, 5.24, 5.15 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.13 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.27 (average value, generator column-GC, Larsen et al. 1992)
5.09 (recommended, Sangster 1993)
5.10 (recommended, Hansch et al. 1995)
5.09, 5.12 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:
7.40 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
log K_{OA} = – 5.41 + 3820/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.58, 7.61 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.40, 7.34 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 3785/(T/K) – 5.35 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
3.83, 3.55, 3.99(algae, fish, act. sludge, Freitag et al. 1984,1985)
2.60–4.08 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.12–5.33 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
3.83, 4.53 (algae: wet wt basis, dry wt basis, Geyer et al. 2000)
3.57, 5.76 (*Daphnia*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
3.90 (soil/sediment, sorption isotherm, Haque & Schmedding 1976)
4.16 (Woodburn silt loam soil, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
4.83 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.90 (Lake Michigan water column, Swackhamer & Armstrong 1987)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
3.99; 4.13 (soil, calculated-Characteristic Root Index CRI; quoted lit., Saçan & Balcioğlu 1996)
4.54–4.56 (Catlin silt loam, f_{OC} = 0.0226, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.65–4.70 (Cloudland loam, f_{OC} = 0.0024, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997
4.61 (Kenoma silt loam, f_{OC} = 0.0153, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.38–4.39 (Kenoma silt loam, f_{OC} = 0.0092, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.57–4.73 (Kenoma silt loam, f_{OC} = 0.002, depth 120–155 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.52–4.54 (Norborne silt loam, f_{OC} = 0.0137, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.54–4.57 (Norborne silt loam, f_{OC} = 0.009, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.53–4.66 (Norborne silt loam, f_{OC} = 0.0057, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.23–4.53; 3.90–5.90 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

4.23; 3.93, 4.53, 4.46 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log K_{OM}:

3.89 (soil organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: depletion rate constant k = 45 d^{-1} from aqueous solution in a 26-cm or 67-cm purge vessel, (Girvin et al. 1997).

Photolysis: photolysis rate k_P(exptl) < 2 × 10^{-8} d^{-1} with $t_{½}$ > 400 d; k_P(calc) < 2 × 10^{-8} d^{-1} in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.4 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = (1.4 – 2.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = (2.0 – 4.2) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, and the k_{OH}(calc) = (1.4 – 3.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Sorption-Desorption Rate Constants:

k_2 = 0.006 d^{-1} with $t_{½}$ = 109 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 104 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: photolysis $t_{½}$ > 400 d in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

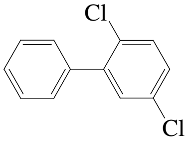
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 109 d for high-dose treatment, $t_{½}$ = 104 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.9 2,5-Dichlorobiphenyl (PCB-9)



Common Name: 2,5-Dichlorobiphenyl
Synonym: PCB-9, 2,5-dichloro-1,1′-biphenyl
Chemical Name: 2,5-dichlorobiphenyl
CAS Registry No: 34883-39-1
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
22–23 (Weingarten 1962)
Boiling Point (°C):
171 (15mm Hg, Erickson 1986))
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
1.0 (calculated, assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.58 (generator column-GC/ECD, Weil et al. 1974)
2.028 (shake flask-GC, Chiou et al. 1977)
0.190 (generator column-GC/ECD, Bruggeman et al. 1981)
1.940 (generator column-GC/ECD, Miller et al. 1984; 1985)
0.0739, 0.0739, 0.0722, 0.07055 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.115 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0775 (Augood et al. 1953)
0.184 (supercooled liquid P_L, Yalkowsky et al. 1983)
0.184 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.202 (GC-RI correlation, Burkhard et al. 1985a)
0.198 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.231, 0.232 (supercooled P_L, GC-RT correlation, different GC stationary phases, Foreman & Bidleman 1985)
0.180 (selected, Shiu & Mackay 1986)
0.204 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -3862/(T/K) + 12.22$, (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.105–0.232 (quoted lit. P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations
39.31 (batch stripping-GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
28.37 (wetted wall column-GC/ECD, Brunner et al. 1990)
16.1, 29.6, 58.2, 82.2, 123, 165.4 (10.4, 20, 30.1, 34.9, 42.1, 47.9°C, gas stripping-HPLC/fluorescence, ten Hulscher et al. 1992)
30.95 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 6.055 - 2331/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

29.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.18	(RP-TLC-k′ correlation, Bruggeman et al. 1982; Bruggeman et al. 1984)
5.16	(generator column-GC/ECD, Miller et al. 1984,1985)
5.03	(calculated-TSA, Burkhard 1984)
4.67; 5.30	(RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
5.01, 5.10, 5.19, 5.10	(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.13	(HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.10	(recommended, Sangster 1993)
5.16	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

8.37, 7.40; 7.33	(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
7.16	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.68	(goldfish, 3% lipid by wt., static fish-water equilibration system, 23-d exposure, Bruggeman et al. 1981)
5.45	(goldfish, 10% lipid dry wt. in food, Bruggeman et al. 1981)
5.72	(guppy, 3.5% lipid by wt., Bruggeman et al. 1982,1984)
4.14; 3.90	(goldfish, exptl.; correlated, Mackay & Hughes 1984)
3.38–4.11 mean 4.00	(rainbow trout, 15°C, steady-state BCF, 7- to 96-d study, Oliver & Niimi 1985)
4.0	(rainbow trout, mean of 7–96 d exposure, Oliver & Niimi 1985)
4.53, 4.00	(rainbow trout: kinetic BCF; steady state BCF, Oliver & Niimi 1985)
4.26	(guppy, Gobas et al. 1987)
5.68	(goldfish, Noegrohati & Hammers 1992)
3.89; 3.42	(zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.0, 5.09	(rainbow trout, flow through 96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.89, 5.43	(zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.00; 4.13	(*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

4.83	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.01	(soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constants k = (0.024–0.038) min^{-1} with $t_{1/2}$ = 18–29 min, k = (0.033–0.048) min^{-1} with $t_{1/2}$ = 14–21 min and k = (0.13–0.14) min^{-1} with $t_{1/2}$ = 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; rate constant k = (0.056–0.064) min^{-1} with $t_{1/2}$ = 11–12 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2; rate constant k = (0.015–0.027) min^{-1} with $t_{1/2}$ = 26–47 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = (1.4 – 2.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = (2.0 – 4.2) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, and the k_{OH}(calc) = (1.4 – 3.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 95% degradation at 24 h in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 920 d^{-1}; k_2 = 0.066 d^{-1} (23°C, goldfish, 3% lipid, Bruggeman et al. 1981; quoted, Waid 1986)
k_2 = 0.008 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 190 d^{-1}; k_2 = 0.11 d^{-1} (guppy, Bruggeman et al. 1984; quoted, Clark et al. 1990)
k_2 = 0.066, 0.0523 d^{-1} (goldfish, exptl., calculated, Mackay & Hughes 1984)
k_1 = 280 d^{-1}; k_2 = 0.0082 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_1 = 38.3, 49.2 h^{-1}; $1/k_2$ = 360, 220 h (goldfish, guppy, quoted, Hawker & Connell 1985)
k_1 = 1200 d^{-1} (guppy, Opperhuizen 1986)
k_1 = 122 d^{-1}; k_2 = 0.0089 d^{-1} (rainbow trout, calculated, Gobas & Mackay 1987)
log k_1 = 2.96, 3.07 d^{-1}; log $1/k_2$ = 0.96, 1.18 d (fish, quoted, Connell & Hawker 1988)
log $1/k_2$ = 2.1, 2.3 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)
log k_2 = – 0.96, –1.17 d^{-1} (fish, quoted, Thomann 1989)
k_1 = 2760 d^{-1}; k_2 = 0.368 d^{-1} (zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{1/2}$ = 192 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.005 d^{-1} with $t_{1/2}$ = 149 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2}$ = 18–29 min, 14–21 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{1/2}$ = 11–12 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2; $t_{1/2}$ = 26–47 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

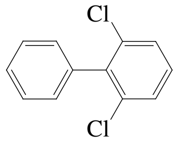
Groundwater:

Sediment:

Soil:

Biota: clearance $t_{1/2}$ = 10 d in goldfish (Bruggeman et al. 1981)
$t_{1/2}$ = 6.5 d in guppy (Bruggeman et al. 1984);
$t_{1/2}$ = 85 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and its muscle, $t_{1/2}$ = 56 d (Niimi & Oliver 1983).
depuration $t_{1/2}$ = 192 d for high-dose treatment, $t_{1/2}$ = 149 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.10 2,6-Dichlorobiphenyl (PCB-10)



Common Name: 2,6-Dichlorobiphenyl
Synonym: PCB-10, 2,6-dichloro-1,1′-biphenyl
Chemical Name: 2,6-dichlorobiphenyl
CAS Registry No: 33146-45-1
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
35.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
12.6 (differential scanning calorimetry, Miller et al. 1984)
Entropy of Fusion, ΔS_{fus} (J/mol K):
41.0 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.789 (mp at 35.5°C)
0.801 Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C):
1.452 (shake flask-GC, Chiou et al. 1977)
1.390 (generator column-GC/ECD, Miller et al. 1984,1985)
0.294, 0.435, 0.245, 0.406 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
2.41 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.540 (generator column-GC/ECD, Opperhuizen et al. 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.288 (GC-RI correlation, Burkhard et al. 1985a)
0.365 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.336, 0.371 (supercooled P_L, GC-RT correlation, different GC stationary phases, Foreman & Bidleman 1985)
0.347 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -3642/(T/K) + 11.74$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
47.83 (calculated-P/C, Burkhard et al. 1985b)
47.61 (calculated-MCI χ, Sabljic & Güsten 1989)
23.30 (wetted wall column-GC, Brunner et al. 1990)
42.86 (calculated-QSPR, Dunnivant et al. 1992)
27.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.30 (quoted, Kaiser 1983)
4.96 (calculated-TSA, Burkhard 1984)
5.31 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.93 (generator column-GC/ECD, Miller et al. 1984,1985)
4.97, 5.00, 4.97, 5.01 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.982 ± 0.013 (shake flask/slow stripping-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
4.99 (recommended, Sangster 1993)
4.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

7.18 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
log $K_{OA} = -4.84 + 3590/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
6.18 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

4.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.99 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: k = 0.043 min^{-1} with $t_{½}$ = 16 min, k = 0.082 min^{-1} with $t_{½}$ = 8 min and k = 0.30 min^{-1} with $t_{½}$ = 2 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; rate constants k = 0.034 min^{-1} with $t_{½}$ = 20 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are: irradiated by sunlight in the presence of 100 µg/mL TiO_2; rate constants k = 0.052 min^{-1} with $t_{½}$ = 13 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 - 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 - 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the k_{OH}(calc) = $(1.4 - 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.004 d^{-1} with $t_{½}$ = 183 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 93 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 16 min, 8 min and 2 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; $t_{½}$ = 20 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{½}$ = 13 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

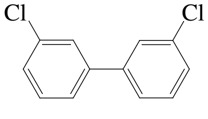
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 56 d for high-dose treatment, $t_{½}$ = 53 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.11 3,3′-Dichlorobiphenyl (PCB-11)



Common Name: 3,3′-Dichlorobiphenyl
Synonym: PCB-11, 3,3′-dichloro-1,1′-biphenyl
Chemical Name: 3,3′-dichlorobiphenyl
CAS Registry No: 2050-67-1
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
29 (Weast 1972–73, 1982–83; Lide 2003)
Boiling Point (°C):
320 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.912 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
1.057 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0406, 0.102, 0.093, 0.0974 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.354 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0267 (P_S from GC-RT correlation, Westcott & Bidleman 1981; Westcott et al. 1981)
0.0865, 0.0952 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
0.0645 (supercooled liquid P_L, GC-RT correlation, Burkhard 1984)
0.0612 (GC-RI correlation, Burkhard et al. 1985a)
0.0646 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.091, 0.076 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.090 (selected P_L, supercooled liquid, Shiu & Mackay 1986)
$\log (P_L/Pa) = -3936/(T/K) + 12.14$; (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0306–0.143; 0.0646–0.0953 (literature. P_S range; literature P_L range, Delle & Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C):
13.58 (calculated-P/C, Burkhard et al. 1985b)
23.61 (batch stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
23.61; 38.69 (quoted exptl.; calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
23.61; 29.42 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.30 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)
5.34 (RP-TLC-k′ correlation, Bruggeman et al. 1982)

5.30, 5.39, 5.22, 5.18 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.17 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.27 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
7.86, 7.90; 7.93 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

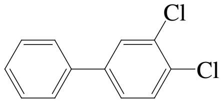
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
4.90 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.00 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 2.7×0^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)
k_{OH} = $(4.1 \pm 1.3) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 297 ± 2 K (relative rate method, Kwok et al. 1995)
tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2: 0.1385 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995)
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 5 d in rainbow trout, and $t_{½}$ < 5 d in its muscle (Niimi & Oliver 1983)

7.1.1.12 3,4-Dichlorobiphenyl (PCB-12)



Common Name: 3,4-Dichlorobiphenyl
Synonym: PCB-12, 3,4-dichloro-1,1′-biphenyl
Chemical Name: 3,4-dichlorobiphenyl
CAS Registry No: 2974-92-7
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
 49–50 (Weingarten 1961)
Boiling Point (°C):
 195–200 (Weast 1972–73)
Density (g/cm^3):
Molar Volume (cm^3/mol):
 226.4 (calculated-Le Bas method at normal boiling point)
 185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
 0.566 (calculated, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
 1.233 (calculated-TSA, supercooled liquid P_L, Burkhard et al. 1985b)
 0.0523, 0.112, 0.0888, 0.128 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 0.00791 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
 0.0138 (supercooled liquid P_L, calculated-mp, Dunnivant & Elzerman 1988)
 0.280 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
 0.091; 0.658 (quoted average of Brodsky & Ballschmiter 1988; calculated- χ, Patil 1991)
 0.4004 (calculated-QSPR, Dunnivant et al. 1992)
 0.930 (calculated-group contribution, Kühne et al. 1995)
 0.268, 0.722 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
 2.373 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
 0.0532 (supercooled liquid P_L, GT-RT correlation, Burkhard 1984)
 0.0313 (GC-RI correlation, Burkhard et al. 1985a)
 0.0532 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985b)
 0.078, 0.062 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 0.741 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
 $\log (P_L/Pa) = -3885/(T/K) + 11.92$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
 0.000736–0.0888; 0.0128–0.0783 (literature P_S range; literature P_L range, Delle Site 1997)
 0.259 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)
 20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Henry's Law Constant (Pa m^3/mol at 25°C):

20.77 (batch stripping/GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
14.18 (wetted-wall column-GC, Brunner et al. 1990)

Octanol/Water Partition Coefficient, log K_{OW}:

5.51 (Hansch & Leo 1979)
5.10, 5,51 (HPLC-RT correlation, calculated-π, Woodburn 1982; Woodburn et al. 1984)
5.29 (generator column-GC, Woodburn et al. 1984)
5.29 (generator column-GC/ECD, Doucette & Andren 1987)
5.26, 5.39, 5.22, 5.18 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.12 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.29 (recommended, Sangster 1993)
5.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

8.71, 7.80; 8.06(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

4.85 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.98 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constants k = (0.019–0.034) min^{-1} with $t_{½}$ = 21–36 min, k = (0.041–0.064) min^{-1} with $t_{½}$ = 11–17 min and k = (0.12–0.16) min^{-1} with $t_{½}$ = 4–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; rate constants k = (0.013–0.029) min^{-1} with $t_{½}$ = 26–52 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.8 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = (1.4 – 2.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = (2.0 – 4.2) × 10^{-12} cm^3 molecule^{-1} s^{-1}, and the calculated k_{OH}(calc) = (1.4 – 3.1) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 100% degraded by Nocardia strain NCIB 10603 within one week (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.010 d^{-1} with $t_{½}$ = 67 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 21–36 min, 11–17 min and 4–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{½}$ = 26–52 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

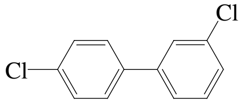
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 88 d for high-dose treatment, $t_{½}$ = 67 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.13 3,4′-Dichlorobiphenyl (PCB-13)



Common Name: 3,4′-Dichlorobiphenyl
Synonym: PCB-13, 3,4′-dichloro-1,1′-biphenyl
Chemical Name: 3,4′-dichlorobiphenyl
CAS Registry No: 2974-90-5
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 233.1
Melting Point (°C):
51 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

1.084	(supercooled liquid S_L, Burkhard et al. 1985a)
0.093	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.369	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.0572	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0595	(GC-RI correlation, Burkhard et al. 1985b)
0.083, 0.067	(supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

log (P_L/Pa) = – 3885/(T/K) + 11.92 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol):

12.36	(calculated-P/C, Burkhard et al. 1985b)
31.92	(calculated-molecular connectivity indices, Sabljic & Güsten 1989)
25.75	(calculated-QSPR, Dunnivant et al. 1992)
49.63	(calculated-QSPR, Achman et al. 1993)
7.44	(11°C, gas stripping-GC/ECD, Bamford et al. 2002)
21.9	(from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 51 \pm 25$ kJ/mol, $\Delta S_H = 0.13 \pm 0.09$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.10	(calculated-TSA, Burkhard 1984)
5.15	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.29	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.15	(recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

7.98	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

4.90 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 2.1 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = (1.4 – 2.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = (2.0 – 4.2) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = (1.4 – 3.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water:

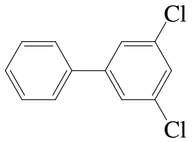
Ground water:

Sediment:

Soil:

Biota:

7.1.1.14 3,5-Dichlorobiphenyl (PCB-14)



Common Name: 3,5-Dichlorobiphenyl
Synonym: PCB-14, 3,5-dichloro-1,1′-biphenyl
Chemical Name: 3,5-dichlorobiphenyl
CAS Registry No: 34883-41-5
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
- 36 (Hinkel & Hay 1928)
- 31–32 (Weingarten 1961; Hutzinger et al. 1974)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
- 226.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
- 0.872 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
- 1.05 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
- 0.00792, 0.0425, 0.0722, 0.109 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 0.128, 0.0662, 0.114 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
- 0.0785 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
- 0.126, 0.117 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- $\log(P_L/\text{Pa}) = -3885/(T/K) + 12.13$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
- 16.72 (calculated-P/C, Burkhard et al. 1985b)
- 49.55 (calculated- QSAR-MCI χ, Sabljic & Güsten 1989)
- 42.63 (calculated-QSPR, Dunnivant et al. 1992)
- 20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
- $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
- 5.37 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)
- 5.63, 5.56, 5.29, 5.16 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.28 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 5.17 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
- 5.41 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
- 8.82, 7.78 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
- 7.53 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.38–3.83 mean 3.79 (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
3.82; 3.79 (rainbow trout: kinetic BCF, steady-state BCF, Oliver & Niimi 1985)

Sorption Partition Coefficient, log K_{OC}:

4.90 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

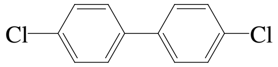
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 2.9×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 - 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)
k_{OH} = $(4.2 \pm 1.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 297 ± 2 K (relative rate method, Kwok et al. 1995)
tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 - 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 - 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 310 d^{-1}; k_2 = 0.046 d^{-1} (rainbow trout, Oliver & Niimi 1985)
log $1/k_2$ = 1.3, 2.5 h (fish, selected, calculated-K_{OW}, Hawker & Connell 1988)
$1/k_2$ = 21.7 d (rainbow trout, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{1/2}$ = 15 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985),
$t_{1/2}$ = 14 d in its muscle (Niimi & Oliver 1983).

7.1.1.15 4,4′-Dichlorobiphenyl (PCB-15)



Common Name: 4,4′-Dichlorobiphenyl
Synonym: PCB-15, 4,4′-dichloro-1,1′-biphenyl
Chemical Name: 4,4′-dichlorobiphenyl
CAS Registry No: 2050-68-2
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
  149.3 (Lide 2003)
Boiling Point (°C):
  317 (Lide 2003)
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
  226.4 (calculated-Le Bas method at normal boiling point)
  185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.059 (Shiu & Mackay 1986)
  0.0546 (Gobas et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
  0.050 (Webb 1970)
  0.060 (Hoover 1971)
  0.080 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
  0.056 (generator column-GC/ECD, Weil et al. 1974)
  0.062 (20°C, shake flask-GC, Chiou et al. 1977; Freed et al. 1977)
  0.046 (generator column-HPLC/UV, Billington 1982)
  0.065 (generator column-HPLC/UV, Huang 1983)
  0.058 (generator column-HPLC/UV, Billington et al. 1988)
  0.151, 0.0774, 0.0952, 0.07055 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  0.0363 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
  0.057 ± 0.0021*(generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
  $\ln x = -2.8677 - 4839.46/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
  1.116, 0.959 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
  $\log S_L/(\text{mol m}^{-3}) = -807/(T/K) + 0.41$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
  $\log S_L/(\text{mol m}^{-3}) = -909/(T/K) + 0.68$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.00253* (Knudsen-effusion technique, extrapolated, Smith et al. 1964)
  0.043 (P_L calculated from P_S using fugacity ratio F, Smith et al. 1964)
  0.071, 0.084 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
  0.0508 (supercooled liquid P_L, Burkhard 1984)
  0.075, 0.059 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.00313 (GC-RI correlation, Burkhard et al. 1985a)
  0.0508 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  0.0263 (extrapolated Antoine eq., Stephenson & Malanowski 1987)

log (P_S/kPa) = – 5416/(T/K) + 12.585; temp range 50–87°C (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 10.10 – 4090/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0603, 0.0776 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 3971/(T/K) + 12.18; (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.00197* (gas saturation-GC/ECD, Wania et al. 1994)
log (P_S/Pa) = – 4977/(T/K) + 14.10; temp range –20 to 30°C (gas saturation-GC, solid, Wania et al. 1994)
0.0426 (supercooled liquid P_L, 20°C, from Falconer & Bidleman, Harner & Bidleman 1996)
0.00313–0.0219; 0518–0.0837 (literature P_S range; literature P_L range, Delle Site 1997)
0.223; 0.084 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI]; quoted lit., Saçan & Balcioğlu 1998)
log P/Pa = 14.10 – 4977/(T/K) temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.0589, 0.0575 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = – 3931/(T/K) + 11.89 (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
log P_L/Pa = – 3829/(T/K) + 11.60 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
30.4 (calculated-P/C, Murphy et al. 1983)
11.04 (calculated-P/C, Burkhard et al. 1985b)
14.69 (calculated, Coates & Elzerman 1986)
17.0 (calculated-P/C, Shiu & Mackay 1986)
20.16 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988)
9.66 (wetted-wall column-GC/ECD, Fendinger & Glotfelty 1990)
18.95; 22.70 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 54 ± 3 kJ/mol, ΔS_H = 0.14 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
14.12, 13.49 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2921/(T/K) + 10.92 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
5.58 (shake flask-GC, Chiou et al. 1977)
5.17 (HPLC-RT correlation, Sugiura et al. 1978)
5.51 (Hansch & Leo 1979)
5.50 (shake flask-GC, Platford 1982)
5.36 ± 0.1; 5.28 (shake flask-GC; RP-TLC-k′ correlation, Bruggeman et al. 1982)
4.92 (HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)
5.33 (generator column-GC/ECD; Woodburn et al. 1984)
4.82 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.30 (selected, Shiu & Mackay 1986)
5.33 (generator column-GC/ECD, Doucette & Andren 1987)
5.03, 5.39, 5.22, 5.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.17 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.23 (recommended, Sangster 1993)
5.58 (recommended, Hansch et al. 1995)
5.35, 5.36 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
7.67* (generator column-GC, measured range – 10 to 20°C, Harner & Mackay 1995)
log K_{OA} = – 5.10 + 3791.7/(T/K), temp range: – 10 to 20°C (generator column-GC, Harner & Mackay 1995)
7.88 (20°C, generator column-GC, Harner & Bidleman 1996)
log K_{OA} = –5.06 + 3792/(T/K); (temp range – 10 to + 20°C, Harner & Bidleman 1996)
8.87, 7.88; 7.89 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

8.12 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.73; 7.77 (calibrated GC-RT correlation, GC-RT correlation, Wania et al. 2002)
7.65, 7.85 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4078/(T/K) – 5.83 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

2.97 (killifish, Goto et al. 1978)
2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
3.47 (calculated-S, Kenaga 1980)
3.58 (rainbow trout, highest value-non-equilibrated, Oliver & Niimi 1984)
4.27 (*picea omorika*, Reischl et al. 1989 from Reischl 1988)
4.06, 5.36 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

4.30 (calculated-solubility, Kenaga 1980)
4.91 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.65 (EPA-B2 river sediment, Coates & Elzerman 1986)
4.03 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated evaporation $t_{½}$ = 4.5 h for an initial concentration of 0.03 ppm in a 4.5 cm depth of water solution in a glass dish and $t_{½}$ = 1.7 h with stirring of the solution; while experimental observed $t_{½}$ = 4.0 h and 1.5 h under the same condition with stirring of the solution (Chiou et al. 1979).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.4 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = (1.4 – 2.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = (2.0 – 4.2) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = (1.4 – 3.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50–80% biodegraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

$t_{½}$ = 72 h for 50% degradation in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, and 55% degradation at 24 h in another PCB mixture by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986);

aerobic biodegradation $t_{½}$ = 1.42 d without the addition of polymer chitin, $t_{½}$ = 0.98 d with chitin and $t_{½}$ = 0.46 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.009 d^{-1} with $t_{½}$ = 81 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 99 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2}$ = 57.5 d in Lake Michigan, 57.5 d (Neely 1983);
aerobic biodegradation $t_{1/2}$ = 1.42 d without the addition of polymer chitin, $t_{1/2}$ = 0.98 d with chitin and $t_{1/2}$ = 0.46 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).
Groundwater:
Sediment:
Soil:
Biota: $t_{1/2}$ = 27 d in *Picea omorika* (Reischl et al. 1989).
depuration $t_{1/2}$ = 81 d for high-dose treatment, $t_{1/2}$ = 99 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.15.1
Reported aqueous solubilities, vapor pressure and octanol-air partition coefficients of 4,4′-dichlorobiphenyl (PCB-15) at various temperatures

Aqueous solubility		Vapor pressure				log K_{OA}	
Shiu et al. 1997		Smith et al. 1964		Wania et al. 1994		Harner & Mackay 1995	
generator column-GC/ECD		Knudsen effusion		gas saturation-GC/ECD		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	log K_{OA}
5	0.021	29.88	0.149	–10	1.206×10^{-5}	–10	9.36
15	0.0346	29.88	0.152	0	8.303×10^{-5}	0	8.83
25	0.0570	66.58	0.504	10	4.159×10^{-4}	10	8.35
35	0.106	66.58	0.432	20	1.197×10^{-3}	20	7.88
45	0.186	76.78	1.26	30	4.475×10^{-3}	25	7.67
		76.78	1.27				
		87.0	3.55	log P/Pa = A – B/(T/K)		ΔH_{OA}/(kJ mol^{-1}) = 72.6	
ΔH_{sol}/(kJ mol^{-1}) = 40.2		87.0	3.57	A	14.10		
	at 5–45°C			B	4977	log K_{OA} = A + B/T	
		log P/mmHg = A – B/(T/K)		temp range –10 to30°C		A	–5.1
		A	13.460			B	3791.7
		B	5416	ΔH_{subl}/(kJ mol^{-1}) = 95.3			

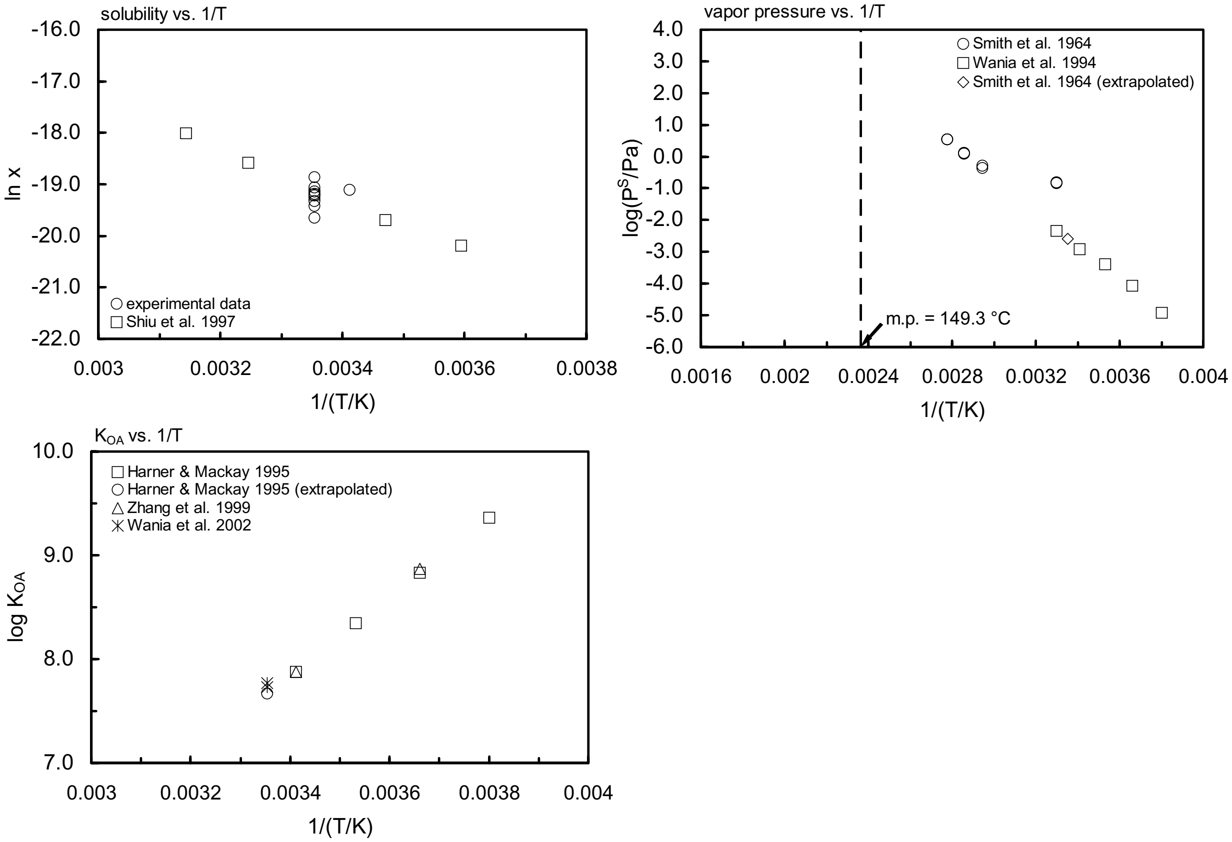
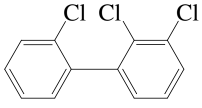


FIGURE 7.1.1.15.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 4,4′-dichlorobiphenyl (PCB-15).

7.1.1.16 2,2′,3-Trichlorobiphenyl (PCB-16)



Common Name: 2,2′,3-Trichlorobiphenyl
Synonym: PCB-16, 2,2′,3-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,3-trichlorobiphenyl
CAS Registry No: 38444-78-9
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
28.1–28.8 (Weingarten 1961; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.934 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.505 (supercooled liquid, calculated-TSA, Burkhard et al. 1985b)
0.293 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.205 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.814 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)
0.674 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0522, 0.066, 0.033 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.069 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.0538, 0.060 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0275 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/mmHg) = 10.10 - 4100/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0427; 0.0427 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -3935/(T/K) + 11.93$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0506; 0.0427 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI; quoted lit., Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
35.16 (calculated-P/C, Burkhard et al. 1985b)
80.0 (calculated-P/C, Shiu & Mackay 1986)
24.11 (20°C, calculated-P/C, Murphy et al. 1987)
81.77 (batch stripping, Atlas et al. 1982)
28.07 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
25.45 (calculated-QSPR, Dunnivant et al. 1992)
4.02, 11.74 (0, 15°C, from modified two-film exchange model, Hornbukle et al. 1994)
9.36 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
25.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 24$ kJ/mol, $\Delta S_H = 0.12 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.36	(calculated-TSA, Burkhard 1984)
4.15	(RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.31	(calculated-π const., Rapaport & Eisenreich 1984)
5.12	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.12	(recommended, Sangster 1993)
5.31	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations.:

7.22; 7.18 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)

$\log K_{OA} = -6.50 + 4240/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)

8.87, 7.98 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)

7.32 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.16	(suspended particulate matter, Burkhard 1984)
6.0	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.52	(soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.00	(soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.7 - 1.6) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\text{-}}(aq.) = 7.2 \times 10^9$ dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(calc) = (1.0 - 2.1) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50% degraded by Nocardia strain NCIB 10603 within 7 d (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.008$ d⁻¹ with $t_{½}$ = 90 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.010$ d⁻¹ with $t_{½}$ = 72 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH· oxidation (Sedlak & Andren 1991)

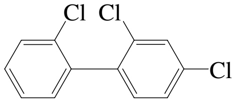
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 90 d for high-dose treatment, $t_{1/2}$ = 72 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.17 2,2′,4-Trichlorobiphenyl (PCB-17)



Common Name: 2,2′,4-Trichlorobiphenyl
Synonym: PCB-17, 2,2′,4-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,4-trichlorobiphenyl
CAS Registry No: 37680-66-3
Molecular Formula: $C_{12}H_8C_2$
Molecular Weight: 257.543
Melting Point (°C):
35 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.292 (supercooled liquid S_L, Burkhard et al. 1985a)
0.259 (supercooled liquid S_L, Murphy et al. 1987)
0.103 (RP-HLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.647 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.080 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0566, 0.0828, 0.0219 (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.0705, 0.0739 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0335 (supercooled liquid P_L, Murphy et al. 1987)
0.0692; 0.0526 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -3935/(T/K) + 12.05$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0692; 0.526 (P_L, quoted lit.; calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
52.18 (calculated-P/C, Burkhard et al. 1985b)
33.03 (calculated-P/C, Murphy et al. 1987)
40.63 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
37.82 (calculated-QSPR, Dunnivant et al. 1992)
26.04 (calculated-QSPR, Achman et al. 1993)
13.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.60, 5.76 (RP-HPLC-RT correlation: uncorrected, with ortho correction, Rapaport & Eisenrich 1984)
5.39 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.50 (generator column-GC, Larsen et al. 1992)

5.50 (recommended, Sangster 1993)
5.76 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
8.06; 7.74 (0; 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

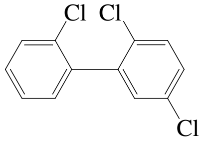
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.24 (suspended particulate matter, Burkhard 1984)
6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.84 (calculated-QSAR-MCI $^1\chi$, Sabljic et al. 1995)
5.20; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH-}(aq.) = 7.5 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.009 d^{-1} with $t_{½}$ = 81 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.007 d^{-1} with $t_{½}$ = 99 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 81 d for high-dose treatment, $t_{½}$ = 99 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.18 2,2′,5-Trichlorobiphenyl (PCB-18)



Common Name: 2,2′,5-Trichlorobiphenyl
Synonym: PCB-18, 2,2′,5-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,5-trichlorobiphenyl
CAS Registry No: 37680-65-2
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
43–44 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.1485
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.648 (Mackay et al. 1980)
0.651 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.640 (shake flask-GC/ECD, Weil et al. 1974)
0.248 (shake flask-GC/ECD, Haque & Schmedding 1975)
0.016 (radioactive isotope-^{14}C labeled, Metcalf et al. 1975)
0.0614 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
0.085 (Kenaga & Goring 1980; Kenaga 1980)
0.110 (shake flask GC/ECD, Bruggeman et al. 1981)
0.299 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.203, 0.135, 0.100, 0.112 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.510; 0.780 (generator column-GC/ECD, supercooled liquid S_L, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.267 (Neely 1981)
0.412 (P_L calculated from P_S using fugacity ratio F, Neely 1981)
0.012 (Neely 1983)
0.0904 (supercooled liquid P_L, Burkhard 1984)
0.0605 (GC-RI correlation, Burkhard et al. 1985a)
0.0904 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985b)
0.0776, 0.0833 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.143; 0.220 (selected: solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
0.0352 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 10.10 - 4090/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0603, 0.0851 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -3935/(T/K) + 12.09$; (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.033–0.0762; 0.035–0.116 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

101.53 (23°C, gas stripping-GC, Atlas et al. 1982)
20.26 (20°C, gas stripping-GC, Oliver 1985)
38.5 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988)
25.33 (wetted-wall column-GC/ECD, Brunner et al. 1990)
8.11, 12.07, 17.64, 25.358* ± 0.34, 34.14 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 9.5020 - 4197.74/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(34.9/\text{kJ}\cdot\text{mol}^{-1})/\ RT] + (0.079/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R]$; where $R = 8.314\ \text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
25.3 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 35 \pm 3$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

3.89 (radiolabeled-^{14}C, Metcalf et al. 1975)
6.22 (shake flask, Hansch & Leo 1979)
5.88 (calculated after Rekker 1977, Könemann 1981)
5.64 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.59; 4.34 (generator column-GC/ECD; HPLC-RT correlation, Woodburn 1982)
4.39, 5.55 (RP-HPLC-RT correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.60; 4.34 (generator column-GC/ECD; HPLC-RT correlation, Woodburn et al. 1984)
4.97 (HPLC-RT correlation, DeVoe et al. 1987)
4.97, 5.68 (HPLC-k′ correlation, De Kock & Lord, 1987)
5.60 (generator column-GC/ECD, Doucette & Andren 1987,1988)
5.31, 5,37, 5,29, 5,37 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.55 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.44 (generator column-GC, Larsen et al. 1992)
5.44 (recommended, Sangster 1993)
5.60 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

7.60; 7.12 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
$\log K_{OA} = -6.00 + 4060/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
8.39 (10°C, estimated, Thomas et al. 1998)
8.70, 7.79 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.48 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.86, 3.76, 2.91, 3.81 (algae, snail, mosquito, fish, ^{14}C-labeled, Metcalf et al. 1975)
1.72 (green sunfish, 15 d in static water, Sanborn et al. 1975)
3.39 (calculated-S, Kenaga 1980)
5.52; 5.83 (goldfish: 10% lipid by wt. in food; 3% lipid, static equilibration system-GC/ECD, 23-d exposure studies, Bruggeman et al. 1981)
3.43–4.23 highest value 4.23 not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
4.91, 4.23; 5.77 (rainbow trout, laboratory data: kinetic BCF(k_1/k_2), steady-state BCF (C_F/C_W); Lake Ontario field BCF, Oliver & Niimi 1985)
4.30 (fish, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
3.75 (*Picea omorika*, Reischl et al. 1989 from Reischl 1988)
4.23 (fish, Isnard & Lambert 1989)
5.82; 5.87 (goldfish; rainbow trout, Noegrohati & Hammers 1992)
4.11; 5.64 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

2.60–4.19 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.08–6.01 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.23, 5.32 (rainbow trout, flow through-96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.30, 5.60 (goldfish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.11, 5.64 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
4.50, 4.50, 5.0 (sediments: offshore Grand Haven 2.0% OC, nearshore Grand Haven 3.4% OC, Benton Harbor sediment 3.8% OC, batch equilibrium-sorption isotherm, Voice et al. 1983; Voice & Weber, Jr., 1985)
5.24 (suspended particulate matter, Burkhard 1984)
5.40; 5.50; 5.20(field data of sediment trap material; Niagara River-organic matter; calculated-K_{OW}, Oliver & Charlton 1984)
5.1–6.3, 5.5; 7.0(suspended sediment, average; algae > 50 µm, Oliver 1987a)
4.57, 4.85 (natural solids, Aldrich humic acid, equilibrium dialysis, Chin & Weber 1989, Chin et al. 1990)
5.34 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.49 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
4.85, 4.15 (Aldrich humic acid substrate with methyl salicylate, organic polymers present in Huron River water, Chin et al. 1990)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.23 (soil, calculated-MCI, Sabljic et al. 1995)
4.53; 4.57 (soil, calculated-Characteristic Root Index [CRI]; quoted lit., Saçan & Balcioğlu 1996)
5.20; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
4.85 (sediment: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH-}(aq.) = 6.9 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{1/2}$~4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 molecule^{-1} s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50–80% being degraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 950 d^{-1}; k_2 = 0.048 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986; Clark et al. 1990)
k_2 = 0.0037 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark 1990)
k_2 = 0.048, 0.0372 d^{-1} (goldfish, exptl., correlated, Mackay & Hughes 1984)
k_1 = 300 d^{-1}; k_2 = 0.0037 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_1 = 39.6 h^{-1}; 1/k_2 = 500 h (goldfish, quoted, Hawker & Connell 1985)
log k_1 = 2.98 d^{-1}; log 1/k_2 = 1.32 d (goldfish, quoted, Connell & Hawker 1988b)
log 1/k_2 = 2.4, 2.4 d (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b).
log 1/k_2 = 1.32 d (goldfish, quoted, Connell & Hawker 1988b; Thomann 1989)
k_1 = 3760 d^{-1}; k_2 = 0.292 d^{-1} (zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.020 d^{-1} with $t_{1/2}$ = 36 d and k_2 = 0.029 d^{-1} with $t_{1/2}$ = 24 d for food concn of 29 ng/g and 182 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_2 = 0.009 d^{-1} with $t_{½}$ = 79 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 96 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 43.1 d in Lake Michigan (Neely 1983); $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991).

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: 0.47 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 1.16 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC,1.21 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.17 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; 0.00838 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 0.00368 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 0.00357 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.00062 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{½}$ = 190 d in rainbow trout, 190 d and its muscle 86 d (Niimi & Oliver 1983);

$t_{½}$ = 190 d in fish (rainbow trout, Niimi & Oliver 1983; Oliver & Niimi 1985);

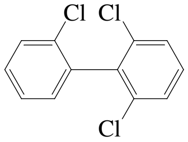
$t_{½}$ = 26 d in worms at 8°C (Oliver 1987c);

$t_{½}$ = 25 d in omorika (Reischl et al. 1989)

Depuration $t_{½}$ = 32–42 d for a 32-d dietary exposure followed by a 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{½}$ = 79 d for high-dose treatment, $t_{½}$ = 96 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.19 2,2′,6-Trichlorobiphenyl (PCB-19)



Common Name: 2,2′,6-Trichlorobiphenyl
Synonym: PCB-19, 2,2′6,-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,6-trichlorobiphenyl
CAS Registry No: 38444-73-4
Molecular Formula: $C_{12}H_7Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
46 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.345 (supercooled liquid S_L, Burkhard et al. 1985a)
0.448 (supercooled liquid S_L, Murphy et al. 1987)
0.447, 0.408, 0.235, 0.246 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.814 (calculated-TSA, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.167 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.171 (GC-RI correlation, Burkhard et al. 1985b)
0.113, 0.131 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0529 (supercooled liquid P_L, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 9.86 - 3970/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0933, 0.138 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -3836/T + 11.93$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
124.6 (calculated-P/C, Burkhard et al. 1985b)
30.70 (calculated-P/C, Murphy et al. 1987)
45.09 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
23.30 (wetted-wall column-GC, Brunner et al. 1990)
44.74 (calculated-QSPR, Dunnivant et al. 1992)
13.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
3.75, 5.48 (RP-HPLC correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
4.88, 5.06, 5.03, 5.19 (RP-HPLC-k′ correction, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.04 (recommended, Sangster 1993)
5.48 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
6.72 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

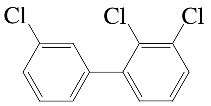
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.28 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.004 d^{-1} with $t_{½}$ = 155 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.008 d^{-1} with $t_{½}$ = 84 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–15 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 155 d for high-dose treatment, $t_{½}$ = 84 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.20 2,3,3′-Trichlorobiphenyl (PCB-20)



Common Name: 2,3,3′-Trichlorobiphenyl
Synonym: PCB-20, 2,3,3′-trichloro-1,1′-biphenyl
Chemical Name: 2,3,3′-trichlorobiphenyl
CAS Registry No: 38444-84-7
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
58 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
337 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.402 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.033 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985a)
0.0283 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0269 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
$\log (P/\text{mmHg}) = 10.40 - 4310/(T/K)$, (GC-RT correlation, Tateya et al. 1988)
0.0302 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4075/(T/K) + 12.12$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry' Law Constant (Pa m^3/mol at 25°C):
81.77 (batch stripping-GC, Atlas et al. 1982)
17.23 (calculated-P/C, Burkhard et al. 1985b)
30.7 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
16.21 (wetted-wall column-GC/ECD, Brunner et al. 1990)
22.01 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.99, 5.57 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.57 (calculated-TSA, Hawker & Connell 1988a)
5.68 (generator column-GC, Larsen et al. 1992)
5.62 (recommended, Sangster 1993)
5.57 (recommended, Hansch et al. 1995)
5.4846 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated:

9.51, 8.49	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.95	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

5.23	(suspended particulate matter, Burkhard 1984)
4.01–4.88; 5.20	(range, calculated from sequential desorption of 11 urban soils; lit. value, Krauss & Wilcke 2001)
5.13; 5.01, 4.88, 5.45	(20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

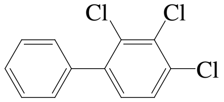
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 88 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.21 2,3,4-Trichlorobiphenyl (PCB-21)



Common Name: 2,3,4-Trichlorobiphenyl
Synonym: PCB-21, 2,3,4-trichloro-1,1′-biphenyl
Chemical Name: 2,3,4-trichlorobiphenyl
CAS Registry No: 55702-46-0
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
101–102 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.176 (mp at 102°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.469 (calculated-TSA, Burkhard et al. 1985b)
0.224, 0.195, 0.142; 0.132 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00489 (GC-RI correlation, Burkhard et al. 1985a)
0.0269 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.0295 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.11$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
14.79 (calculated-P/C, Burkhard et al. 1985b)
21.38 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
23.0 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.88 (calculated after Rekker 1977, Könemann 1981)
5.77 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.51, 5.61, 5.87, 5.73 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.860 ± 0.017(slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990;)
5.68 (recommended, Sangster 1993)
5.86 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.16 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}

5.19 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constants k = 0.021 min^{-1} with $t_{1/2}$ = 33 min, k = 0.059min^{-1} with $t_{1/2}$ = 12 min and $t_{1/2}$ = 0.14 min^{-1} with $t_{1/2}$ = 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; rate constants k = 0.0050 min^{-1} with $t_{1/2}$ = 139 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2}$ = 33 min, 12 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{1/2}$ = 139 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

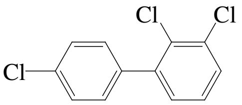
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.22 2,3,4′-Trichlorobiphenyl (PCB-22)



Common Name: 2,3,4′-Trichlorobiphenyl
Synonym: PCB-22, 2,3,4′-trichloro-1,1′-biphenyl
Chemical Name: 2,3,4′-trichlorobiphenyl
CAS Registry No: 38444-85-8
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
73 (Burkhard et al. 1985a; Shiu & Mackay 1986; Brodsky & Ballschmiter 1988)
69.0 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.335 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.397 (supercooled liquid S_L, Burkhard et al. 1985b)
0.142 (supercooled liquid S_L, Murphy et al. 1987)
0.408 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0696 (calculated-QSPR, Dunnivant et al. 1992)
0.187 (calculated-group contribution method, Kühne et al. 1995)
0.0677, 0.178 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.469 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0239 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0084 (GC-RI correlation, Burkhard et al. 1985b)
0.026, 0.023 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0111 (supercooled liquid P_L, Murphy et al. 1987)
0.0191, 0.0263(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.08$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0478 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C):
15.40 (calculated-P/C, Burkhard et al. 1985b)
20.16 (calculated-P/C, Murphy et al. 1987)
14.18 (wetted-wall column-GC/ECD, Brunner et al. 1990)
22.60 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
25.03; 19.35 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)
13.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
31.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 31 \pm 1$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

4.84, 5.42 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.29 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.63 (generator column-GC, Larsen et al. 1992)
5.45 (recommended, Sangster 1993)
5.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.60; 8.58 (0; 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.70, 4.90 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.24 (suspended particulate matter, Burkhard 1984)
6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.90 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 7.4 × 10^9 dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.012 d⁻¹ with $t_{½}$ = 56 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.011 d⁻¹ with $t_{½}$ = 64 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

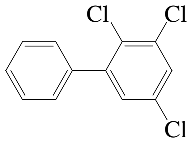
Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 56 d for high-dose treatment, $t_{½}$ = 64 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.23 2,3,5-Trichlorobiphenyl (PCB-23)



Common Name: 2,3,5-Trichlorobiphenyl
Synonym: PCB-23, 2,3,5-trichloro-1,1′-biphenyl
Chemical Name: 2,3,5-trichlorobiphenyl
CAS Registry No: 55720-44-0
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
41 (Burkhard et al. 1985a)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.694 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.402 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.223 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0402 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0291 (GC-RI correlation, Burkhard et al. 1985b)
0.0447 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4075/(T/\text{K}) + 12.36$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
25.74 (calculated-P/C, Burkhard et al. 1985a)
35.6 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
32.26 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.44 (calculated-TSA, Burkhard 1984)
5.53 (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
5.57 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.6729 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.23 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

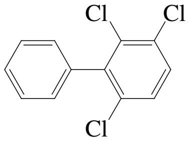
Ground water:

Sediment:

Soil:

Biota:

7.1.1.24 2,3,6-Trichlorobiphenyl (PCB-24)



Common Name: 2,3,6-Trichlorobiphenyl
Synonym: PCB-24, 2,3,6-trichloro-1,1′-biphenyl
Chemical Name: 2,3,6-trichlorobiphenyl
CAS Registry No: 55702-45-9
Molecular Formula: $C_{12}H_7Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
49 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.581 (mp at 49°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.507 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.132 (20°C, supercooled liquid, Murphy et al. 1987)
0.0677, 0.118, 0.0604, 0.098 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.514 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.167; 0.136, 0.358 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.132; 0.853 (quoted exptl., calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.087 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0899 (GC-RI correlation, Burkhard et al. 1985b)
0.0166 (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/mmHg) = 10.6 - 4090/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0708 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -3935/(T/K) + 12.02$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
44.18 (calculated-P/C, Burkhard et al. 1985a)
32.12 (20°C, Murphy et al. 1987)
34.35 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
22.3 (wetted-wall column-GC, Brunner et al. 1990)
31.53 (calculated-QSPR, Dunnivant et al. 1992)
14.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

4.52, 5.67 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.45, 5.42, 5.44, 5.46 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.44 (recommended, Sangster 1993)
5.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

7.75 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.16 (suspended particulate matter, Burkhard 1984)
6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: k = (0.019–0.029) min^{-1} with $t_{½}$ = 24–36 min, k = (0.041–0.059) min^{-1} with $t_{½}$ = 12–17 min and k = (0.12–0.22) min^{-1} with $t_{½}$ = 3–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; rate constants, k = (0.0066–0.030) min^{-1} with $t_{½}$ = 23–105 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are: irradiated by sunlight in the presence of 100 μg/mL TiO_2; rate constant k = 0.022 min^{-1} with $t_{½}$ = 31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 7.6 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.009 d^{-1} with $t_{½}$ = 81 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime τ = 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime τ = 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);

$t_{½}$ = 24–36 min, 12–17 min and 3–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{½}$ = 23–105 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 μg/mL TiO_2; $t_{½}$ = 31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

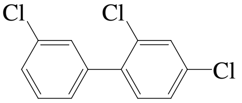
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 81 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.25 2,3′,4-Trichlorobiphenyl (PCB-25)



Common Name: 2,3′,4-Trichlorobiphenyl
Synonym: PCB-25, 2,3′,4-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,4-trichlorobiphenyl
CAS Registry No: 55712-37-3
Molecular Formula: $C_{12}H_3H_7$
Molecular Weight: 257.543
Melting Point (°C):
61 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.317 (supercooled liquid S_L, Burkhard et al. 1985a)
0.025 (supercooled liquid S_L, Murphy et al. 1987)
0.20 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.1025 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0313 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0327 (GC-RI correlation, Burkhard et al. 1985b)
0.0373, 0.0366 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.24×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0295, 0.0372(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4075/(T/\text{K}) + 12.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
25.53 (calculated-P/C, Burkhard et al. 1985a)
43.27 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
32.04 (calculated-QSPR, Dunnivant et al. 1992)
17.20 (calculated-QSPR, Achman et al. 1993)
14.0 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.51 (calculated-TSA, Burkhard 1984)
5.67 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.54 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.63 (calculated, Miertus & Jakus 1990)
5.54 (recommended, Sangster 1993)
5.6793 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.31; 8.28; 8.23(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

7.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.31 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 7.2 × 10^9 dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.008 d⁻¹ with $t_{½}$ = 87 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d⁻¹ with $t_{½}$ = 102 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

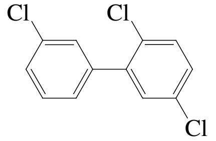
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 87 d for high-dose treatment, $t_{½}$ = 102 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.26 2,3′,5-Trichlorobiphenyl (PCB-26)



Common Name: 2,3′,5-Trichlorobiphenyl
Synonym: PCB-26, 2,3′,5-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,5-trichlorobiphenyl
CAS Registry No: 38444-81-4
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
  40.0–40.5 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  247.3 (calculated-Le Bas method at normal boiling point)
  198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.705 (mp at 40.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.219, 0.166, 0.205, 0.155 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  0.253 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
  0.138 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.0353 (supercooled liquid P_L, Burkhard et al. 1984)
  0.0262 (GC-RI correlation, Burkhard et al. 1985a)
  0.0363 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  0.0411, 0.0412 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.0182 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  0.0316, 0.389 (supercooled liquid P_L, GC-RI correlation, different stationary phases Fischer et al. 1992)
  $\log (P_L/Pa) = -4075/(T/K) + 12.28$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
  0.0112–0.0402; 0.0182–0.0449 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C):
  32.93 (gas stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
  20.27 (wetted-wall column-GC, Brunner et al. 1990)
  12.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  30.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  5.76 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
  5.52, 5.68, 5,72, 5,68 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  5.65 (recommended, Sangster 1993)
  5.76 (recommended, Hansch et al. 1995):

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.30, 8.27; 8.24(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

8.57 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.31 (suspended particulate matter, Burkhard 1984)

6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\text{-}}$(aq.) = 6.3 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 from lake sediments but small residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.007 d^{-1} with $t_{½}$ = 105 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 135 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

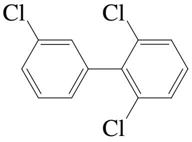
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 105 d for high-dose treatment, $t_{½}$ = 135 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.27 2,3′,6-Trichlorobiphenyl (PCB-27)



Common Name: 2,3′,6-Trichlorobiphenyl
Synonym: PCB-27, 2,3′,6-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,6-trichlorobiphenyl
CAS Registry No: 38444-81-4
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
45 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.404 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.039 (supercooled liquid S_L, Murphy et al. 1987)
0.256 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0653 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0676 (GC-RI correlation, Burkhard et al. 1985b)
0.0598, 0.0628 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.26×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0490, 0.0708 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -3935/(T/K) + 11.97$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C or as indicated):
41.64 (calculated-P/C, Burkhard et al. 1985a)
49.95 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
41.0 (calculated-QSPR, Dunnivant et al. 1992)
22.17 (quoted as PCB-24 and 27, Achman et al. 1993)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.43 (calculated-TSA, Burkhard 1984)
5.44 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.52 (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
5.50 (quoted as PCB-24 and 27, Murray & Andren 1992)
5.2417 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
7.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.23	(suspended particulate matter, Burkhard 1984)
6.40	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.7–1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 7.6×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(1.0–2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.008$ d^{-1} with $t_{½} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.009$ d^{-1} with $t_{½} = 81$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

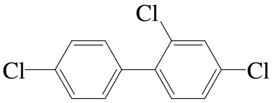
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 81 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.28 2,4,4′-Trichlorobiphenyl (PCB-28)



Common Name: 2,4,4′-Trichlorobiphenyl
Synonym: PCB-28, 2,4,4′-trichloro-1,1′-biphenyl
Chemical Name: 2,4,4′-trichlorobiphenyl
CAS Registry No:7012-37-5
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
57–58 (Hutzinger et al. 1971,1974)
Boiling Point (°C):
206–207 (Sengupta 1966)
Density (g/cm^3 at 20°C): 1.1485
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.6 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.482 (Mackay et al. 1980; Shiu & Mackay 1986)
0.482 (Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.085 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.260 (generator column-GC/ECD, Weil et al. 1974)
0.119 (Dexter & Pavlou 1978)
0.270 (20°C, supercooled liquid S_L, shake flask-GC/ECD, Chiou et al.1983; Chiou 1985)
0.142 (generator column-HPLC/UV, Huang 1983)
0.163 (generator column-GC/ECD, Miller et al. 1984)
0.312 (supercooled liquid P_L, calculated-TSA, Burkhard et al. 1985b)
0.116 (shake flask-GC/ECD, Chiou et al. 1986)
0.143 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixture, Murphy et al. 1987)
0.177, 0.107, 0.144,0.117 (RP-HPLC-k′ correlation, different stationary and mobile Brodsky & Ballschmiter 1988)
0.067 (22°C, generator column-GC, Opperhuizen et al. 1988)
0.117 (generator column-GC, Dunnivant & Elzerman 1988)
log [S_L/(mol/L)] = 0.232 – 975.5/(T/K); (supercooled liquid, Passivirta et al. 1999)
0.260, 0.228 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S_L/(mol m^{-3}]) = – 1147/(T/K) + 0.79 (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0277 (supercooled liquid P_L, Burkhard 1984)
0.014 (GC-RI correlation, Burkhard et al. 1985a)
0.0277 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0339, 0.0340(supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0149 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0277, 0.0335(supercooled liquid, Dunnivant & Elzerman 1988)
log (P/mmHg) = 10.40 – 4270/(T/K) (GC-RT correlation, Tateya et al. 1988)

0.257, 0.0324(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4075/(T/K) + 12.20 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0210; 0.0436(solid, supercooled liquid, Passivirta et al. 1999)
log (P_S/Pa) = 15.15 – 5049/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 12.20 – 4075/(T/K) (supercooled liquid, Passivirta et al. 1999)
0.0234, 0.0269(supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log (P_L/Pa) = – 4157/(T/K) + 12.31 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log (P_L/Pa) = – 4007/(T/K) + 11.87 (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations
32.02 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
8.7, 21.2, 47.4, 50.3, 70.8, 120.6, 122.2 (10.4, 20, 30.1, 34.9, 42.1, 47.9, 48.4°C, gas stripping-HPLC/fluorescence, ten Hulscher et al. 1992)
log [H/(Pa·m^3/mol)] = 11.97 – 3100/(T/K); (Passivirta et al. 1999)
13.13, 19.06, 27.18, 38.14 ± 0.37, 50.39 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
K_{AW} = exp[– (32.5/kJ·mol^{-1})/ RT] + (0.074/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
19.72 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 6.324 – 2467/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
36.5 (exptl. data, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 33 ± 2 kJ/mol, ΔS_H = 0.07 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
33.11, 30.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2010/(T/K) + 857 (LDV linear regression of literature data, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2860/(T/K) + 11.08 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
4.38 (shake flask-GC, Paris et al. 1978)
5.74 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.62 (shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
5.69 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.51, 5.77, 5.81, 5.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.68 (generator column-GC, Larsen et al. 1992)
5.59 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.71 (recommended, Sangster 1993)
5.62 (recommended, Hansch et al. 1995)
5.55, 5.66 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
7.92 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
log K_{OA} = – 6.12 + 4190/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.76 (10°C, estimated, Thomas et al. 1997)
9.43, 8.40 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.03 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.93, 7.85 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4102/(T/K) – 5.91 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
2.60–3.82 (various marine species, mean dry wt. BCF, Hope et al. 1998)
3.82–4.93 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.32, 5.62 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.74, 5.66 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.50, 4.70 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

4.23 (calculated, Kenaga 1980)
4.38 (log K_{OM} soil organic matter, Wood burn soil, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
5.31 (suspended particulate matter, Burkhard 1984)
5.28 (sediment: suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
5.30; 4.59 (suspended solids-Lake Superior: calculated-K_{OW}, Baker et al. 1986)
4.40; 3.54 (Sanhedron soil-Suwannee River; humic acid, shake flask-GC, Chiou et al. 1986, 1987)
3.89; 3.57 (Sanhedron soil-Suwannee River; fulvic acid, shake flask-GC, Chiou et al. 1986, 1987)
4.84; 4.24 (Fluka-Tridom humic acid; Calcasieu River humic extract, Chiou et al. 1987)
3.53; 3.27 (Suwannee River water sample; Sopchoppy River water sample, Chiou et al. 1987)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.03–4.91; 5.30–5.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.25; 5.27, 4.91, 5.32 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolysis rate k_P(exptl) = 6×10^{-8} d^{-1} with $t_{½}$ = 133 d; k_P(calc) = 2.2×10^{-8} d^{-1} in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 7.2×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{½}$ = 7 h of biodegradation by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

49% degradation at 72 h in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.016 d^{-1} with $t_{½}$ = 44 d and k_2 = 0.015 d^{-1} with $t_{½}$ = 46 d for food concn of 16 ng/g and 108 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_1 = 0.00054 h^{-1}; k_2 = 0.089 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)

k_1(calc) = 11 (food lipid (mg)/(g worm lipid-d); k_2(calc) = 0.14 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995);

$t_{1/2}$ = 72 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis $t_{1/2}$ = 133 d in winter sunlight at 40°L in surface waters (Dulin et al. 1986);

half-lives range from $t_{1/2} \sim$ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);

$t_{1/2}$ = 1450 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{1/2}$ = 26000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: 0.47 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 1.15 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 1.34 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.53 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; 0.00378 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 0.00183 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 0.0016 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.00044 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

$t_{1/2}$ = 26000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

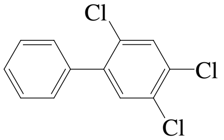
Biota: depuration $t_{1/2}$ = 44–46 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$t_{1/2}$ = 7.8 h in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination $t_{1/2}$ = 5 d in earthworm given contaminated food (predicted, Wågman et al. 2001)

depuration $t_{1/2}$ = 91 d for high-dose treatment, $t_{1/2}$ = 88 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.29 2,4,5-Trichlorobiphenyl (PCB-29)



Common Name: 2,4,5-Trichlorobiphenyl
Synonym: PCB-29, 2,4,5-trichloro-1,1′-biphenyl
Chemical Name: 2,4,5-trichlorobiphenyl
CAS Registry No: 15862-07-4
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
78.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.1485
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22.8 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
65.27 (Miller et al. 1984)
65.24, 63.0 (literature exptl. value, calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.30 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.092 (generator column-GC/ECD, Weil et al. 1974)
0.119 (Dexter & Pavlou 1978)
0.140 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)
0.142 (generator column-HPLC/UV, Huang 1983)
0.162 (generator column-GC/ECD, Miller et al. 1984, 1985)
0.0.098, 0.107,0.138,0.120 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.106* ± 0.0045 (generator column-GC/ECD, Shiu et al. 1997)
0.0413, 0.0682, 0.106, 0.203, 0.33 (5, 15, 25, 35, 45°C, generator column-GC, Shiu et al. 1997)
$\ln x = -3.06175 - 4633.86/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.479, 0.389 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -824/(T/K) + 0.03$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -977/(T/K) + 0.46$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0443 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.0112 (GC-RI correlation, Burkhard et al. 1985a)
0.0320 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0453, 0.0464 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4075/(T/K) + 12.20$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0263 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994; Harner & Bidleman 1996)
0.0447, 0.0457 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/Pa = -3904/(T/K) + 11.75$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
20.27 (wetted-wall column-GC, Brunner et al. 1990; quoted, Achman et al. 1993)
37.89* ± 0.53 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 9.863 - 4197.74/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(34.9/kJ{\cdot}mol^{-1})/\ RT] + (0.082/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where $R = 8.314\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
36.3 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 35 \pm 3$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
32.36, 30.20 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -1674/(T/K) + 7.13$ (LDV linear regression of literature data, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -2927/(T/K) + 11.30$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations:
6.22 (Hansch & Leo 1979)
5.77 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.86 (HPLC-RT correlation, Woodburn 1982)
5.51 (generator column-GC/ECD, Miller et al. 1984)
5.81 (generator column-GC, Woodburn et al. 1984)
5.86 (HPLC-RT correlation, Woodburn et al. 1984)
6.25 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.66 (HPLC-RP/MS, Burkhard & Kuehl 1986)
5.81 (generator column-GC/ECD, Doucette & Andren 1987)
5.78, 5.82, 5.88, 5,76 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.86 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
5.901 ± 0.007 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.54 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.81 (recommended, Sangster 1993)
5.90 (recommended, Hansch et al. 1995)
5.74, 5.60 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
7.96* (generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)
$\log K_{OA} = -4.80 + 3791.7/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Mackay 1995)
8.03 (20°C, generator column-GC, Harner & Bidleman 1996)
$\log K_{OA} = -4.77 + 3792/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
9.15, 8.05 (0, 20°C, multi-column GC-k′ correlation; Zhang et al. 1999)
8.21 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.01; 8.03 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
7.80, 7.78 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4175/(T/K) - 6.22$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
4.97 (guppy, lipid wt. based, Gobas et al. 1989)
5.41 (guppy, corr. lipid wt. based, Gobas et al. 1989)
4.36, 5.53 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
5.26 (suspended particulate matter, Burkhard 1984)
4.51 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constants k = (0.019–0.022) min^{-1} with $t_{½}$ = 31–36 min, k = (0.033–0.048) min^{-1} with $t_{½}$ = 14–21 min and k = (0.13–0.14) min^{-1} with $t_{½}$ = 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; rate constants k = (0.0056–0.020) min^{-1} with $t_{½}$ = 35–123 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: half-life of biodegradation by *Alcaligenes* sp. strain Y-42 from lake sediments estimated to be less than 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

log k_2 = – 1.68 d^{-1} (fish, quoted, Hawker & Connell 1985; Thomann 1989)

k_2 = 0.004 d^{-1} with $t_{½}$ = 190 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 100 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 31–36 min, 14–21 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{½}$ = 35–123 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 190 d for high-dose treatment, $t_{½}$ = 100 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.29.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficient log of 2,4,5-trichlorobiphenyl (PCB-29) at various temperatures

Solubility		Henry's law constant		log K_{OA}	
Shiu et al. 1997		Bamford et al. 2000		Harner & Mackay 1995	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
5	0.0413	4	12.12	–10	9.5
15	0.0682	11	18.04	0	8.97
25	0.106	18	28.37	10	8.51
35	0.203	25	37.89	20	8.03
45	0.330	31	51.03	25	7.96
		$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		ΔH_{OA}/(kJ mol^{-1}) = 72.6	
ΔH_{sol}/(kJ mol^{-1}) = 36.9			K_{AW}		
at 5–45°C		A	9.8629	$\log K_{OA} = A + B/T$	
		B	4197.74	A	–4.8
		enthalpy, entropy change:		B	3791.7
		ΔH/(kJ·mol^{-1}) = 34.9 ± 2.8			
		ΔS/(J·mol^{-1}·K^{-1}) = 82 ± 10			

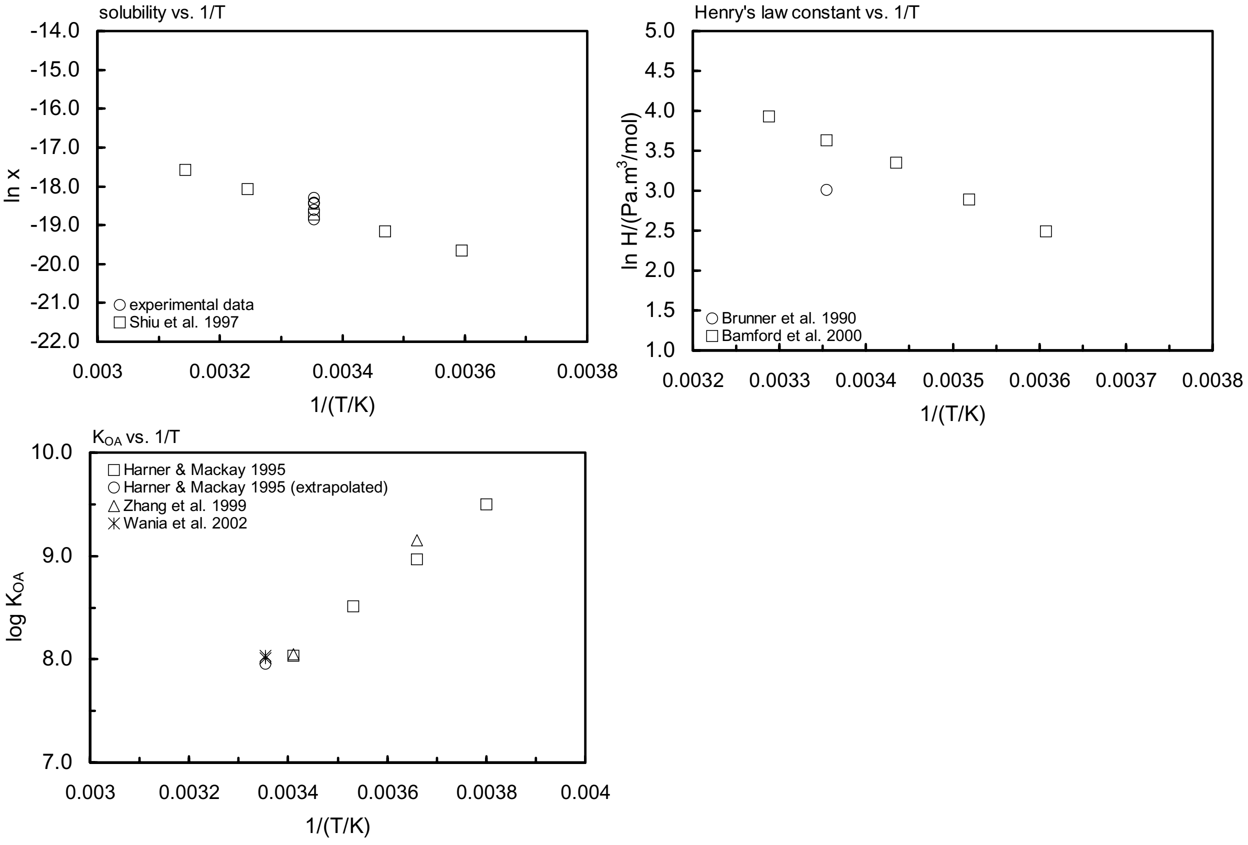
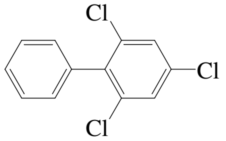


FIGURE 7.1.1.29.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,4,5-trichlorobiphenyl (PCB-29).

7.1.1.30 2,4,6-Trichlorobiphenyl (PCB-30)



Common Name: 2,4,6-Trichlorobiphenyl
Synonym: PCB-30
Chemical Name: 2,4,6-trichlorobiphenyl
CAS Registry No: 35693-92-6
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
62.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
16.5 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999))
Entropy of Fusion, ΔS_{fus} (J/mol K):
49.37 (Miller et al. 1984)
49.36, 63.0 (literature exptl. value, calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F :
0.427 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.226 (generator column/ECD, Miller et al. 1984,1985)
0.024, 0.0468, 0.0491, 0.0893 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.187* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988)
0.0803, 0.187, 0.435 (4, 25, 40°C, generator column-GC/ECD, Doucette & Andren 1988)
$S/(mol/L) = 2.49 \times 10^{-7} \exp(0.047 \cdot t/°C)$ (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
$\log x = -1742/(T/K) - 1.983$, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
0.252, 0.243 (generator column-GC, Dunnivant & Elzerman 1988)
0.236 (generator column-GC, Li et al. 1992)
0.235 (generator column-GC/ECD, Li et al. 1993)
0.217 (shake flask-GC/ECD, Li & Andren 1994)
$\ln x = -4.5969 - 4004.7/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.031 (Augood 1953; quoted, Bidleman 1984)
0.0865, 0.0948(P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.030 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
0.0955, 0.144(supercooled liquid P_L calculated from P_{GC}, GC-RT correlation, different stationary phases, Bidleman 1984)
0.0421 (GC-RI correlation, Burkhard et al. 1985a)
0.111, 0.135 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0946 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.110; 0.0851(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -3886/(T/K) + 12.02$; (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0130–0.0637; 0.085–0.146 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C):

61.40 (calculated-P/C, Burkhard et al. 1985b)
49.51 (calculated-P/C, Shiu & Mackay 1986)
65.76 (batch stripping, Dunnivant et al. 1988 Dunnivant & Elzerman 1988)
47.51 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
58.04 (calculated-QSPR, Dunnivant et al. 1992)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.47 (generator column-GC/ECD, Miller et al. 1984, 1985)
5.57 (generator column-GC/ECD, Doucette & Andren 1987,1988)
5.77, 5.70, 5.51, 5.48 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.33, 5.57 (RP-HPLC-k′ correlation, different stationary phases, Sherblom & Eganhouse 1988)
5.711 ± 0.014 (shake flask/slow stirring, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.75 (generator column-GC, Li et al. 1993)
5.62 (recommended, Sangster 1993)
5.71 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

7.28 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.24 (suspended particulates matter, Burkhard 1984)
4.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

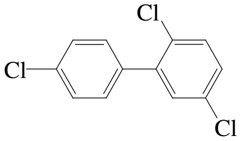
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 molecule^{-1} s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation: 30% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

7.1.1.31 2,4′,5-Trichlorobiphenyl (PCB-31)



Common Name: 2,4′,5-Trichlorobiphenyl
Synonym: PCB-31, 2,4′,5-trichloro-1,1′-biphenyl
Chemical Name: 2,4′,5-trichlorobiphenyl
CAS Registry No: 16606-02-3
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
67 (Bellavita 1935; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.384 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.11 (Kilzer et al. 1979)
0.075 (shake flask-GC/ECD, Bruggeman et al. 1981)
0.265, 0.155, 0.179, 0.120 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.090 (generator column-GC/ECD, Opperhuizen et al. 1988)
0.143 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.220, 0.194 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -1123/(T/K) + 0.64$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0341, 0.0474 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
0.0132 (GC-RI correlation, Burkhard et al. 1985a)
0.0313 (supercooled liquid P_L, calculated-GC-RI correlation, Burkhard et al. 1985b)
0.0373, 0.0346 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0149 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 10.40 - 4270/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0263, 0.0347 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4058/(T/K) + 12.14$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.024, 0.0257 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log (P_L/\text{Pa}) = -4149/(T/K) + 12.29$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log (P_L/\text{Pa}) = -4010/(T/K) + 11.86$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
94.13 (gas-stripping-GC, Atlas et al. 1982)
20.26 (calculated, Murphy et al. 1983)
25.43 (calculated-P/C, Burkhard et al. 1985b)
26.75 (20°C, calculated-P/C, Murphy et al. 1987)

28.47 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
19.25 (wetted-wall column-GC/ECD, Brunner et al. 1990)
27.78 (calculated-QSPR, Dunnivant et al. 1992)
20.21 (calculated-QSPR, Achman et al. 1993)
12.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
30.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
37.15, 33.88 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(\text{Pa m}^3/\text{mol})] = -2887/(T/K) + 11.22$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.22 (Hansch & Leo 1979)
5.30 (HPLC-RT correlation, Woodburn 1982; Woodburn et al.1984)
5.77 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.69 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.79 (generator column-GC/ECD, Woodburn et al. 1984)
5.70 (selected, Shiu & Mackay 1986)
5.99, 6.22, 6.18, 6.33 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.79 (generator column-GC/ECD, Doucette & Andren 1987,1988)
5.59 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.68 (recommended, Sangster 1993)
5.79 (recommended, Hansch et al. 1995)
5.79, 5.78 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:
7.92 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
$\log K_{OA} = -6.12 + 4190/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
9.43, 8.40; 8.23 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.93, 7.94 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4110/(T/K) - 5.84$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
3.45 (fish, Korte et al. 1978)
– 0.30, – 0.22 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
6.15 (goldfish, 3% lipid, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
5.98 (goldfish, 10% lipid content in food, Bruggeman et al. 1981)
3.95, 3.95, 4.51 (algae, fish, activated sludge, Freitag et al. 1984,1985)
3.66 (salmon fry in humic water-steady state, Carlberg et al. 1986)
3.83 (salmon fry in lake water-steady state, Carlberg et al. 1986)
4.62 (fish, calculated-C_B/C_W or k_1/k_2 Connell & Hawker 1988; Hawker 1990)
4.66; 6.19 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4/09 (algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)
5.04 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
3.95, 4.65 (algae: wet wt basis, dry wt basis, Geyer et al. 2000)
4.23, 5.23 (*Daphna*: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.08, 6.04 (mussel: wet wt basis, dry wt basis, Geyer et al. 2000)
4.63, 5.93 (goldfish: wet wt basis, dry wt basis, Geyer et al. 2000)
4.67, 6.19 (zebrafish: wet wt basis, dry wt basis, Geyer et al. 2000

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.90, 4.80 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.31 (suspended particulates, Burkhard 1984)

5.5–6.3, 5.9; 6.80 (suspended sediment, average; algae > 50 μm, Oliver 1987a)

5.48 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)

4.63 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)

5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

4.51 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

5.10 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\text{-}}$(aq.) = 7.2 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 molecule^{-1} s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Biodegradation: 50–80% being degraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 890 d^{-1}; k_2 = 0.021 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986)

k_2 = 0.0035 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

k_1 = 37.1 h^{-1}; 1/k_2 = 1142 h (goldfish, quoted, Hawker & Connell 1985)

log k_1 = 2.95 d^{-1}; log 1/k_2 = 1.68 d (fish, quoted, Connell & Hawker 1988; Thomann 1989)

k_1 = 3950 d^{-1}; k_2 = 0.0867 d^{-1} (zebrafish, 30-d exposure, Fox et al. 1994)

k_1 = 5044 h^{-1}, k_2 = 0.411 h^{-1} (algae *Chlorella fusca*, Wang et al. 1996)

k_1 = 0.00447 h^{-1}; k_2 = 0.100 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)

k_1 = 14 L d^{-1} g^{-1} dry wt.; k_2 = 0.129 d^{-1} (Baltic Sea blue mussels, flow-through expt. Gustafsson et al. 1999)

k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from, $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

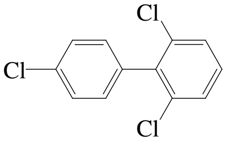
Groundwater:

Sediment:

Soil:

Biota: $t_{1/2}$ = 196 d in rainbow trout, and $t_{1/2}$ = 81d in its muscle, (Niimi & Oliver 1983);
- $t_{1/2}$ = 30 d in worms at 8°C (Oliver 1987c);
- theoretical half-life to reach 90% steady-state tissue concn 5.4 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);
- $t_{1/2}$ = 6.9 h in blood plasma (ring doves, Drouillard & Norstrom 2000).
- depuration $t_{1/2}$ = 91 d for high-dose treatment, $t_{1/2}$ = 88 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.32 2,4′,6-Trichlorobiphenyl (PCB-32)



Common Name: 2,4′,6-Trichlorobiphenyl
Synonym: PCB-32, 2,4′,6-trichloro-1,1′-biphenyl
Chemical Name: 2,4′,6-trichlorobiphenyl
CAS Registry No: 38444-77-8
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
70 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.399 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.355, 0.182, 0.129, 0.0778 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0578 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.060 (GC-RI correlation, Burkhard et al. 1985b)
0.0543, 0.0562(supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P/mmHg) = 16.10 - 4100/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0427, 0.0589(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -3935/(T/K) + 11.93$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
37.29 (calculated-P/C, Burkhard 1984)
41.75 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
39.69 (calculated-QSPR, Dunnivant et al. 1990)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.60, 5.75 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.80 (selected, Shiu & Mackay 1986)
4.95, 5.29, 5.21, 5.52 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.47 (generator column-GC, Larsen et al. 1992)
5.49 (recommended, Sangster 1993)
5.75 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

7.72 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)

log K_{OA} = –6.50 + 4240/(T/K); temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)

8.89, 7.97; 7.92 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al 1999)

7.49 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.23 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 8.0 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.008 d^{-1} with $t_{½}$ = 85 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.006 d^{-1} with $t_{½}$ = 111 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

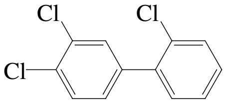
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 85 d for high-dose treatment, $t_{½}$ = 111 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.33 2,3′,4′-Trichlorobiphenyl (PCB-33)



Common Name: 2,3′,4′-Trichlorobiphenyl
Synonym: PCB-33, 2,3′,4′-trichlorobiphenyl, 2′,3,4-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,4′-trichlorobiphenyl
CAS Registry No: 38444-86-9
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
60–60.5 (Wallnöfer et al. 1973)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.1485
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.452 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.078 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.291 (calculated-TSA, Mackay et al. 1980)
0.0796 (quoted lit. average, Yalkowsky et al. 1983)
0.371 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b;)
0.246, 0.170, 0.103, 0.142 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0814 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.133 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.103 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)
0.152 (calculated-QSPR, Dunnivant et al. 1992)
0.209 (calculated-group contribution, Kühne et al. 1995)
0.0833, 0.219 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.576 (calculated–mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0107 (P_S from GC-RT correlation, Westcott & Bidleman 1981)
0.0133, 0.0160 (solid P_S, 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
log (P_S/mmHg) = 1.09 – 1510/(T/K), temp range 30–40°C (gas saturation-GC/ECD, Westcott et al. 1981)
0.030 (P_L calculated from P_S using fugacity ratio F, Westcott et al. 1981)
0.0115 (GC-RI correlation, Burkhard et al. 1985a)
0.0243 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0264, 0.0219 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0136, 0.030 (selected P_S, P_L, Shiu & Mackay 1986)
0.0119 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P_L/mmHg) = 10.40 – 4330/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0137; 0.0272 (quoted; calculated-UNIFAC, Banerjee et al. 1990)
0.0214, 0.0295(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)

log (P_L/Pa) = – 4075/(T/K) + 12.09 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.00484–0.0270; 0.0119–0.030 (quoted lit. P_S range; lit. P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
15.20 (calculated, Murphy et al. 1983)
16.92 (calculated-P/C, Burkhard et al. 1985b)
43.67 (calculated-P/C, Shiu & Mackay 1986)
22.70 (20°C, calculated-P/C, Murphy et al. 1987)
21.99 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
16.21 (wetted wall column-GC,/ECD, Brunner et al. 1990)
24.31 (calculated-QSPR, Dunnivant et al. 1992)
11.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
29.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 42 ± 22 kJ/mol, ΔS_H = 0.11 ± 0.08 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.48, 5.66, 5.98, 5.71 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.872 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.71 (recommended, Sangster 1993)
5.87 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
9.52, 8.52 (0, 20°C, multi-column GC-k′ correlation; Zhang et al. 1999)
8.03 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
3.79 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)
3.79, 6.04 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.57, 5.87 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
5.26 (suspended particulate matter, Burkhard 1984)
4.64 (soil, calculated-S, Chou & Griffin 1986)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.20 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH^-}(aq.) = 7.2 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 molecule^{-1} s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.008\ d^{-1}$ with $t_{½} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008\ d^{-1}$ with $t_{½} = 88$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½} \sim 4–11$ d in freshwater systems, $t_{½} = 0.1–10$ d in cloud water, $t_{½} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

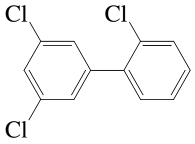
Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 1.90\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.88\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.37\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00413\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00099\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00052\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: depuration $t_{½} = 91$ d for high-dose treatment, $t_{½} = 88$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.34 2,3′,5′-Trichlorobiphenyl (PCB-34)



Common Name: 2,3′,5′-Trichlorobiphenyl
Synonym: PCB-34, 2,3′,5′-trichlorobiphenyl, 2,3′,5′-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,5′-trichlorobiphenyl
CAS Registry No: 37680-68-5
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
58.0 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.474 (mp at 58°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.319 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.129 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.205 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.036 (P_L supercooled liquid, Burkhard et al. 1985a)
0.0177 (GC-RI correlation, Burkhard et al. 1985b)
0.0447 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.37$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
29.08 (calculated-P/C, Burkhard 1984)
51.17 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
42.73 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.51 (calculated-TSA, Burkhard 1984)
5.66 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.71 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988; recommended, Sangster 1993)
5.6522 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
7.72 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.31 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

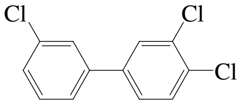
Ground water:

Sediment:

Soil:

Biota:

7.1.1.35 3,3′,4-Trichlorobiphenyl (PCB-35)



Common Name: 3,3′,4-Trichlorobiphenyl
Synonym: PCB-35
Chemical Name: 3,3′,4-trichlorobiphenyl
CAS Registry No: 37680-69-6
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
87.0 (Burkhard et al. 1985a)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.246 (mp at 87°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.301 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0152 (quoted-3,4,4′-trichlorobiphenyl from Weil et al. 1974; Opperhuizen et al. 1988)
0.0814 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.0514 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00246 (GC-RI correlation, Burkhard et al. 1985a)
0.00949 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.014, 0.0105 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0129 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4242/(T/K) + 12.37$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
8.13 (calculated-P/C, Burkhard et al. 1985b)
22.49 (calculated-MCI χ, Sabljic & Güsten 1989)
18.23 (calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.53 (calculated-TSA, Burkhard 1984)
5.82 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.7151 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.85 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.33 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

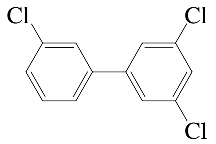
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.36 3,3′,5-Trichlorobiphenyl (PCB-36)



Common Name: 3,3′,5-Trichlorobiphenyl
Synonym: PCB-36, 3,3′,5-trichloro-1,1′-biphenyl
Chemical Name: 3,3′,5-trichlorobiphenyl
CAS Registry No: 38444-87-0
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
46 (estimated, Abramowitz & Yalkowsky)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.260 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.00469, 0.0155, 0.010 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0814 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0141 (P_L supercooled liquid, Burkhard et al. 1985a)
0.0149 (GC-RI correlation, Burkhard et al. 1985b)
0.0191 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4242/(T/\text{K}) + 2.48$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
13.98 (calculated-P/C, Burkhard et al. 1985a)
51.47 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
17.40 (wetted-wall column-GC/ECD, Brunner et al. 1990)
34.10 (calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.57 (calculated-TSA, Burkhard 1984)
4.15 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
5.70 (selected, Shiu & Mackay 1986)
5.88 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.76, 5.86, 5.80 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.81 (recommended, Sangster 1993)
5.8293 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

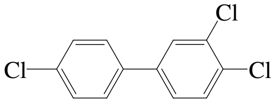
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.37 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:

7.1.1.37 3,4,4′-Trichlorobiphenyl (PCB-37)



Common Name: 3,4,4′-Trichlorobiphenyl
Synonym: PCB-37
Chemical Name: 3,4,4′-trichlorobiphenyl
CAS Registry No: 38444-90-5
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
86.8–87.8 (Weingarten 1961)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.244 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0152 (generator column-GC/ECD, Weil et al. 1974)
0.135 (calculated-TSA, Mackay et al. 1980)
0.296 (supercooled liquid, calculated-TSA, Burkhard et al. 1985b)
0.0853 (calculated-fragment solubility constants, Wakita et al. 1986)
0.072 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0110, 0.0142, 0.00853, 0.853 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0408 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.0287 (calculated-QSPR, Dunnivant et al. 1992)
0.0437, 0.115 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.170 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0566, 0.00897, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0084 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.0127, 0.0094 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00454 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00912, 0.0115 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4242/(T/K) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0612 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
84.21 (batch stripping, Atlas et al. 1982)
7.34 (calculated-P/C, Burkhard et al. 1985b)
15.40 (20°C, calculated-P/C, Murphy et al. 1987)
14.59 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
15.41 (calculated-QSPR, Dunnivant et al. 1992)

20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.90 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.00 (calculated-fragment const., Yalkowsky et al. 1983)
5.53 (calculated-TSA, Burkhard 1984)
4.94 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.58, 5.86, 5.84, 5.85 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.83 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.78 (recommended, Sangster 1993)
5.7373 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

8.97 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.58, 5.90 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.70, 4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.33 (suspended particulate matter, Burkhard 1984)
4.81 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.81 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
4.46 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

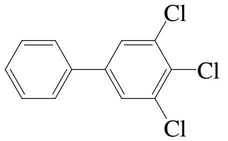
Environmental Fate Rate Constants or Half-Lives:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

7.1.1.38 3,4,5-Trichlorobiphenyl (PCB-38)



Common Name: 3,4,5-Trichlorobiphenyl
Synonym: PCB-38, 3,4,5-trichloro-1,1′-biphenyl
Chemical Name: 3,4,5-trichlorobiphenyl
CAS Registry No: 53555-66-1
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
114 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.353 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0258 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0104 (P_L supercooled liquid, Burkhard et al. 1985a)
0.0566, 0.0111, 0.0219 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
7.62 (calculated-P/C, Burkhard 1984)
20.97 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
2.027 (wetted-wall column-GC/ECD, Brunner et al. 1990)
23.54 (calculated-QSPR, Dunnivant et al. 1992)
19.30 (calculated-QSPR, Achman et al. 1993)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 54 ± 3 kJ/mol, ΔS_H = 0.14 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.48 (calculated-TSA, Burkhard 1984)
5.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.7298 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.92 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.28 (suspended particulate matter, cal-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

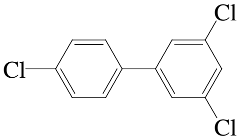
Ground water:

Sediment:

Soil:

Biota:

7.1.1.39 3,4′,5-Trichlorobiphenyl (PCB-39)



Common Name: 3,4′,5-Trichlorobiphenyl
Synonym: PCB-39, 3,4′,5-trichloro-1,1′-biphenyl
Chemical Name: 3,4′,5-trichlorobiphenyl
CAS Registry No: 38444-88-1
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):

88	(Burkhard et al. 1985b)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

247.3	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.241 (mp at 88°C)

Water Solubility (g/m^3 or mg/L at 25°C):

0.353	(supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.0258	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0310	(calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.0125 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0135, 0.00314, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.0203, 0.0174 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/\text{Pa}) = -4242/(T/\text{K}) + 12.53$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

12.56	(calculated-P/C, Burkhard et al. 1985a)
43.57	(calculated-molecular connectivity indices, Sabljic & Güsten 1989)
30.32	(calculated-QSPR, Dunnivant et al. 1992)
20.3	(predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 54 ± 3 kJ/mol, ΔS_H = 0.14 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.58	(calculated-TSA, Burkhard 1984)
5.89	(calculated-TSA, Hawker & Connell 1988a quoted, Hansch et al. 1995)
5.8173	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

8.79	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.38	(suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

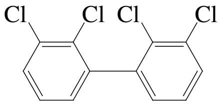
Ground water:

Sediment:

Soil:

Biota:

7.1.1.40 2,2′,3,3′-Tetrachlorobiphenyl (PCB-40)



Common Name: 2,2′,3,3′-Tetrachlorobiphenyl
Synonym: PCB-40
Chemical Name: 2,2′,3,3′-tetrachlorobiphenyl
CAS Registry No: 38444-93-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
  119.5–121.5 (Wallnöfer et al. 1973; Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
  268.2 (calculated-Le Bas method at normal boiling point)
  211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.113 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
  0.034 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
  0.070, 0.0583, 0.0232, 0.0385 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  0.0156 (generator column-GC/ECD; Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  0.0098 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
  0.00134 (GC-RI correlation, Burkhard et al. 1985a)
  0.0112 (supercooled liquid P_L, GC-RI correlation, Burkhard et al.)
  0.00887, 0.00861 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.00255; 0.0020 (selected solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
  0.00452 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  log (P/mmHg) = 10.70 – 4480/(T/K) (GC-RT correlation, Tateya et al. 1988)
  0.00676, 0.012(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
  log (P_L/Pa) = –4271/(T/K) + 12.32 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
  0.000473–0.00957; 0.00450–0.0120 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
  20.27 (calculated-P/C, Burkhard et al. 1985b;)
  12.16 (20°C, batch stripping-GC, Oliver 1985)
  21.94 (calculated-P/C, Shiu & Mackay 1986)
  16.31 (20°C, calculated-P/C, Murphy et al. 1987)
  20.47 (batch stripping-GC, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
  45.14 (calculated-QSAR-χ, Sabljic & Güsten 1989)
  10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
  18.52 (calculated-QSPR, Dunnivant et al. 1992)
  15.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)

29.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

4.63 (HPLC-RT correlation, Sugiura et al. 1978)
5.56 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.80 (shake flask-GC, Chiou 1985)
5.48, 5.66, 5.84, 5.85 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.55 (generator column-GC/ECD, Hawker & Connell 1988a)
6.178 (slow stirring-GC; De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.67 (recommended, Sangster 1993)
6.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

8.05 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.08 (killifish, Goto et al. 1978)
3.36–4.23 highest value 4.23 not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
4.69, 4.23; 5.38 (rainbow trout: laboratory data: kinetic BCF; steady state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
4.38, 4.23 (worms, fish, Oliver 1987c)
4.23 (fish, quoted, Isnard & Lambert 1988, 1989)

Bioaccumulation Factor, log BAF:

6.48 (rainbow trout, L/kg(lp), quoted, Thomann 1989)

Biota Sediment Accumulation Factor, BSAF:

10 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:

5.57 (suspended particulate matter, Burkhard 1984)
5.50; 5.50 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
5.00 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
5.00 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 6.1×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0065\ d^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 320\ d^{-1}$; $k_2 = 0.0065\ d^{-1}$ (rainbow trout, Oliver & Niimi 1985)

log $1/k_2$ = 2.2, 2.9 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)

$k_2 = 0.006\ d^{-1}$ with $t_{½} = 107$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.006\ d^{-1}$ with $t_{½} = 112$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½} = 0.1$–10 d in cloud water, $t_{½} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.20\ d^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.95\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.36\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.39\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; $k = 0.00155\ d^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00285\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00258\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00119\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

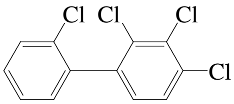
Biota: half-life in rainbow trout, $t_{½} = 107$ d and $t_{½} = 61$ d its muscle (Niimi & Oliver 1983);

$t_{½} = 107$d in rainbow trout (Oliver & Niimi 1985);

$t_{½} = 29$ d in worms at 8°C (Oliver 1987c).

depuration $t_{½} = 107$ d for high-dose treatment, $t_{½} = 112$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.41 2,2′,3,4-Tetrachlorobiphenyl (PCB-41)



Common Name: 2,2′,3,4-Tetrachlorobiphenyl
Synonym: PCB-41, 2,2′,3,4-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4-tetrachlorobiphenyl
CAS Registry No: 52663-59-9
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
63 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.150 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.0648 (20°C, supercooled liquid S_L, Murphy et al. 1987)
0.0306, 0.0328, 0.0197, 0.0351 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.116 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0124 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0131 (GC-RI correlation, Burkhard et al. 1985b)
0.0110, 0.0098 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.59×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0776, 0.0120(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.22$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
23.91 (calculated-P/C, Burkhard et al. 1984)
20.37 (calculated-P/C, Murphy et al. 1987)
20.87 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
14.19 (wetted-wall column-GC, Brunner et al. 1990; quoted, Achman et al. 1993)
24.76 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.09, 6.11 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.73, 5.83, 5.82, 5.78 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.79 (recommended, Sangster 1993)
6.11 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.79, 8.82	(0, 20°C, RP-HPLC-RT, Zhang et al. 1999)
8.46	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.59	(suspended particulate matter, Burkhard 1984)
5.01	(soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.40	(soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 6.4×10^9 dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.005 d⁻¹ with $t_{½}$ = 147 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d⁻¹ with $t_{½}$ = 162 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

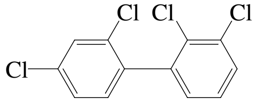
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 147 d for high-dose treatment, $t_{½}$ = 162 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.42 2,2′,3,4′-Tetrachlorobiphenyl (PCB-42)



Common Name: 2,2′,3,4′-Tetrachlorobiphenyl
Synonym: PCB-42, 2,2′,3,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′-tetrachlorobiphenyl
CAS Registry No: 36559-22-5
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
 69.0 (Burkhard et al. 1985; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
 268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol 9K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.370 (mp at 69°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.150	(supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.0608	(20°C, supercooled liquid S_L, Murphy et al. 1987)
0.032	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0923	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0334	(calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.0131	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00507	(GC-RI correlation, Burkhard et al. 1985b)
0.0116, 0.0116	(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.19×10^{-3}	(20°C, supercooled liquid, Murphy et al. 1987)

 log (P/mmHg) = 10.70 – 4480/(T/K) (GC-RT correlation, Tateya et al. 1988)
 0.00912, 0.0135 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
 log (P_L/Pa) = –4229/(T/K) + 12.25 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

29.49	(calculated-P/C, Burkhard et al. 1985a)
32.02	(calculated-molecular connectivity indices, Sabljic & Güsten 1989)
14.19	(wetted-wall column-GC, Brunner et al. 1990)
25.92	(calculated-QSPR, Dunnivant et al. 1995)
10.13	(calculated-QSPR, Achman et al. 1993)
21.4	(11°C, gas stripping-GC/ECD, Bamford et al. 2002)
38.0	(from 11°C exptl. data and compensation point, Bamford et al. 2002)

 ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 3$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.84	(calculated-TSA, Burkhard 1984)
5.76	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.72	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.72	(quoted values; recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

9.19	(10°C, estimated, Thomas et al. 1998)
8.27	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.64	(suspended particulate matter, Burkhard 1984)
5.30	(soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4 – 0.9) × 10^{-12} cm³ molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} cm³ molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.006 d^{-1} with $t_{½}$ = 123 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 140 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

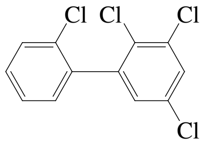
Ground water:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.20 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.89 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.23 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.35 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; k = 0.00066 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00309 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.0016 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00101 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: depuration $t_{½}$ = 123 d for high-dose treatment, $t_{½}$ = 140 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.43 2,2′,3,5-Tetrachlorobiphenyl (PCB-43)



Common Name: 2,2′,3,5-Tetrachlorobiphenyl
Synonym: PCB-43
Chemical Name: 2,2′,3,5-tetrachlorobiphenyl
CAS Registry No: 70362-46-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.130 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.146 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0183 (P_L supercooled liquid, Burkhard et al. 1985a)
0.0194 (GC-RI correlation, Burkhard et al. 1985b)
0.0166, 0.0191 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0123, 0.0191 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.40$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
41.14 (calculated-P/C, Burkhard 1984)
35.26 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
33.94 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated-TSA, Burkhard 1984)
5.75 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8627 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.64 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{½}$ = 155 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 188 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

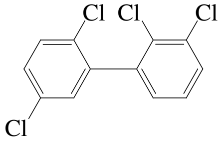
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 155 d for high-dose treatment, $t_{½}$ = 188 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.44 2,2′,3,5′-Tetrachlorobiphenyl (PCB-44)



Common Name: 2,2′,3,5′-Tetrachlorobiphenyl
Synonym: PCB-44
Chemical Name: 2,2′,3,5′-tetrachlorobiphenyl
CAS Registry No: 41464-39-5
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
46.5–47 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.608 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.170 (shake flask-GC, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.080 (generator column-HPLC/UV, Billington 1982)
0.10 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.08 (generator column-HPLC/UV, Billington et al. 1988)
0.0463, 0.0394, 0.0254, 0.0343 (RP-HPLC-k′ correlation correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00943 (GC-RI correlation, Burkhard et al. 1985a)
0.0147 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0128, 0.013 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0152 (quoted, Eisenreich 1987)
0.0064 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00955, 0.0151 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.29$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
79.28 (batch stripping, Atlas et al. 1982)
24.32 (calculated, Murphy et al. 1983)
32.83 (calculated-P/C, Burkhard et al. 1985b)
19.15 (20°C, calculated-P/C, Murphy et al. 1987)
25.43 (calculated-QSPR-MCI χ, Sabljic & Gusten 1989)
14.19 (wetted-wall column-GC, Brunner et al. 1990)
23.32 (calculated-QSPR, Dunnivant et al. 1992)
11.86, 16.02, 21.33, 28.05* ± 0.27, 35.13 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 5.8937 - 3103.2/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(25.8/\text{kJ·mol}^{-1})/RT] + (0.049/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where $R = 8.314\ \text{J·K}^{-1}\text{·mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)—see Comment by Goss et al. 2004
27.0 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.67 (calculated-fragment const., Yalkowsky et al. 1983)
5.84 (calculated-TSA, Burkhard 1984)
5.81 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.29 (calculated-S, Chou & Griffin 1986)
5.61, 5.78, 5.74, 5.79 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.75 (calculated-TSA, Hawker & Connell 1988b)
5.88 (calculated-MCI χ, Patil 1991)
5.73 (recommended, Sangster 1993)
5.81 (recommended, Hansch et al. 1995)
6.20, 4.79–6.67 (calculated-Characteristic Root Index [CRI]; minimum-maximum range, Saçan & Inel 1995)
5.6625 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.26 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:
8.36 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
$\log K_{OA} = -6.20 + 4340/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
9.19 (10°C, estimated, Thomas et al. 1998)
9.67, 8.71; 8.41 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.58 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
4.04 (oyster, Vreeland 1974)
4.84; 6.37 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.04, 6.29 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.84, 5.37 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.60, 4.70 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
5.64 (suspended particulate matter, Burkhard 1984)
4.43 (soil, calculated-S, Chou & Griffin 1986)
5.60 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.67 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.05 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
5.40 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH^-}(aq.) = 5.5 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation: 99% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 200 d^{-1}; k_2 = .0461 d^{-1} (Zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.014 d^{-1} with $t_{½}$ = 49 d and k_2 = 0.018 d^{-1} with $t_{½}$ = 38 d for food concn of 18 ng/g and 129 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_2 = 0.005 d^{-1} with $t_{½}$ = 146 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 175 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:

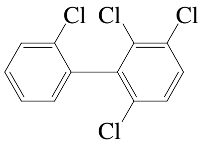
Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.23 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.98 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.32 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.38 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; k = 0.00090 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00253 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00161 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00122 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: depuration $t_{½}$ = 38–49 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{½}$ = 146 d for high-dose treatment, $t_{½}$ = 175 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.45 2,2′,3,6-Tetrachlorobiphenyl (PCB-45)



Common Name: 2,2′,3,6-Tetrachlorobiphenyl
Synonym: PCB-45, 2,2′,3,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,6-tetrachlorobiphenyl
CAS Registry No: 70362-45-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.115 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.146 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.292 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0398 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0416 (GC-RI correlation, Burkhard et al. 1985b)
0.0226, 0.0268 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0295 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4117/(T/K) + 12.16$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
101.1 (calculated-P/C, Burkhard 1984)
31.92 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
35.95 (calculated-QSPR, Dunnivant et al. 1992)
12.47 (calculated-QSPR, Achman et al. 1993)
25.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
43.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.88 (calculated-TSA, Burkhard 1984)
5.53 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
4.84 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988
4.84 (recommended, Sangster 1993)
5.4616 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.28 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.68 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 6.7×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 7 food lipid (mg)/(g worm lipid-d); k_2 = 0.12 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 175 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 128 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Ground water:

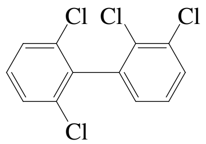
Sediment:

Soil:

Biota: elimination $t_{½}$ = 6 d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{½}$ = 175 d for high-dose treatment, $t_{½}$ = 128 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.46 2,2′,3,6′-Tetrachlorobiphenyl (PCB-46)



Common Name: 2,2′,3,6′-Tetrachlorobiphenyl
Synonym: PCB-46, 2,2′,3,6′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,6′-tetrachlorobiphenyl
CAS Registry No: 41464-47-5
Molecular Formula: $C_{12}H_6H_4$
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.114 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.106 (20°C, supercooled liquid, Murphy et al. 1987)
0.149 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0280 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0272 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0285 (GC-RI correlation, Burkhard et al. 1985b)
0.0186, 0.0206 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.04×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0155 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4229/(T/\text{K}) + 12.37$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
69.81 (calculated-P/C, Burkhard 1984)
26.04 (20°C, calculated-P/C, Murphy et al. 1987)
36.68 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
34.33 (calculated-QSPR, Dunnivant et al. 1992)
18.87 (calculated-QSAR, Achman et al. 1993)
18.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
34.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.89 (calculated-TSA, Burkhard 1984)
5.53 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
4.84 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.86 (calculated, Miertus & Jakus 1990)

4.84	(recommended, Sangster 1993)
5.2787	(calculated-molecular properties MNDO-AM1 method, Makino 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.49, 8.56	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1998)
7.91	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.69	(suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.006 d^{-1} with $t_{½}$ = 112 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.006 d^{-1} with $t_{½}$ = 907 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

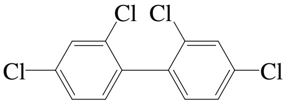
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 112 d for high-dose treatment, $t_{½}$ = 107 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.47 2,2′,4,4′-Tetrachlorobiphenyl (PCB-47)



Common Name: 2,2′,4,4′-Tetrachlorobiphenyl
Synonym: PCB-47
Chemical Name: 2,2′,4,4′-tetrachlorobiphenyl
CAS Registry No: 2437-79-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
83 (Fichter & Adler 1926; Kühne et al. 1995; Ruelle & Kesselring 1997)
41–42 (Hall & Minhaj 1957; Wallnöfer et al. 1973)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.268 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.068 (shake flask-GC, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.990 (supercooled liquid S_L, Johnstone et al. 1974)
0.0160, 0.0157, 0.0172, 0.0202 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0541 (22°C, generator column-GC, Opperhuizen et al. 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0115 (Neely 1983)
0.0111 (GC-RI correlation, Burkhard et al. 1985a)
0.0151 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0152, 0.0156 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0115, 0.0162 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4229/(T/\text{K}) + 12.37$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
42.86 (calculated-P/C, Burkhard et al. 1985b)
17.38 (calculated-P/C, Shiu & Mackay 1986)
44.48 (calculated-QSAR- χ, Sabljic & Güsten 1989)
19.25 (wetted-wall column-GC/ECD, Brunner et al. 1990)
37.30 (calculated-QSPR, Dunnivant et al. 1992)
3.05, 8.91 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
12.67 (estimated-bond method, EPIWIN v3.04, Hardy 2002)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.68 (shake flask, Tulp & Hutzinger 1978)
5.20 (HPLC-k′ correlation, McDuffie 1981)

6.29 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.17 (HPLC-k′ correlation, De Kock & Lord 1987)
5.93, 6.04, 5.86, 5.94 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.94 (recommended, Sangster 1993)
6.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
9.55, 8.56 (0, 20°C, multi-column GC-k′ correlation; Zhang et al. 1999)
8.01 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
3.98 (rainbow trout muscle, steady state, Branson et al. 1975; quoted, Waid 1986)
4.09 (rainbow trout, Neely et al. 1974)
3.95 (rainbow trout, Branson et al. 1975)
4.85; 4.782, 4.717 (quoted-whole fish; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
2.97, 2.71 (phytoplankton *Nanochloropsis oculata*, PCB concn at 50 ppb, after 4-d culture, Wang et al. 1998)
2.19, 2.11 (phytoplankton *Isochrysts galbana*, PCB concn at 500 ppb, after 4-d culture, Wang et al. 1998)
4.00, 5.52 (rainbow trout 8–10 g, muscle 3% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.46, 5.56 (rainbow trout 10–15 g, whole fish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.76 (estimated-EPIWIN v3.04, Hardy 2002)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.30, 4.70 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
4.61 (soil, calculated-solubility, Kenaga 1980)
5.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.68 (soil, calculated-S, Chou & Griffin 1986)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.04 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.70 (soil, calculated-K_{OW}, Girvin & Scott 1997)
4.65 (estimated-EPIWIN v3.04, Hardy 2002)

Sorption Partition Coefficient, log K_P:
5.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.18–5.64 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2}$ = 0.2921 d from river, $t_{1/2}$ = 9.256 d from lake (estimated-EPIWIN v3.04, Hardy 2002).
Photolysis: photolysis rate $k_P = 0.553\ d^{-1}$ with $t_{1/2}$ = 13 d in summer sunlight; k_P(exptl) = $6 \times 10^{-8}\ d^{-1}$ with $t_{1/2}$ = 133 d, and k_P(calc) = $2.2 \times 10^{-8}\ d^{-1}$ in winter sunlight, at 40°L in surface waters (Dulin et al. 1986)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH\text{-}}$(aq.) = $6.4 \times 10^9\ dm^3\ mol^{-1}\ s^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–0 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: no degradation observed after 98 d incubation by river dieaway test (Bailey et al. 1983).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 286\ d^{-1}$; $k_2 = 0.030\ d^{-1}$ (10–12°C, rainbow trout muscle, Branson et al. 1975; quoted, Waid 1986)

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 160$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 177$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 49.2$ d in Lake Michigan (Neely 1983);

photolysis $t_{1/2} = 13$ d in summer sunlight and $t_{1/2} = 170$ d in winter sunlight at 40°L in surface waters (Dulin et al. 1986);

half-lives range from $t_{1/2} \sim 4$–11 d in freshwater systems, $t_{1/2} = 0.1$–10 d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);

half-life of volatilization: $t_{1/2} = 0.2021$ d from river, and $t_{1/2} = 9.156$ d from lake, (estimated-EPIWIN v3.04, Hardy 2002).

Groundwater:

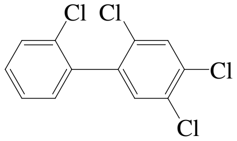
Sediment:

Soil:

Biota: $t_{1/2} = 28$ d in rainbow trout muscle (Branson et al. 1975; selected, Waid 1986).

depuration $t_{1/2} = 160$ d for high-dose treatment, $t_{1/2} = 177$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.48 2,2′,4,5-Tetrachlorobiphenyl (PCB-48)



Common Name: 2,2′,4,5-Tetrachlorobiphenyl
Synonym: PCB-48, 2,2′,4,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5-tetrachlorobiphenyl
CAS Registry No: 70362-47-9
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
65.9 (Miller et al. 1984; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.4 (Miller et al. 1984; Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
69.04 (Miller et al. 1984)
Fugacity Ratio at 25°C, F:
0.393 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.121 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.030 (supercooled liquid S_L, Murphy et al. 1987)
0.0328, 0.0376, 0.0467, 0.0452 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0222, 0.0596 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0167 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985a)
0.0177 (ΔG_v and GC-k′ correlation, Burkhard et al. 1985b)
0.0157, 0.016 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0265 (20°C, supercooled liquid, Murphy et al. 1987)
0.0115, 0.0170 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.37$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.010 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI; Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
42.71 (calculated-P/C, Burkhard et al. 1985b)
26.64 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
30.67 (calculated-QSPR, Dunnivant et al. 1992)
19.30 (calculated-QSPR, Achman et al. 1993)
3.05, 8.91 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
22.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
39.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.86 (calculated-TSA, Burkhard 1984)
5.78 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.71, 5.79, 5.56 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.95 (calculated-solvatochromic parameters and intrinsic molar volume V_I, Kamlet et al. 1988)
5.69 (recommended, Sangster 1993)
5.9108 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.49, 8.50 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

4.41, 5.71 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.66 (suspended particulate matter, Burkhard 1984)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

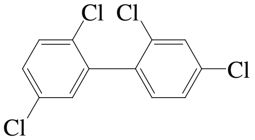
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.4 – 0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH\text{-}}$(aq.) = 6.4 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.004 d^{-1} with $t_{1/2}$ = 160 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{1/2}$ = 177 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{1/2}$ = 160 d for high-dose treatment, $t_{1/2}$ = 177 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.49 2,2′,4,5′-Tetrachlorobiphenyl (PCB-49)



Common Name: 2,2′,4,5′-Tetrachlorobiphenyl
Synonym: PCB-49, 2,2′,4′,5-tetrachlorobiphenyl, 2,2′,4,5′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5′-tetrachlorobiphenyl
CAS Registry No: 41464-40-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
66.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.4 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
69.04 (Miller et al. 1984)
69.01, 64.3 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.392 (mp at 66.5°C)
0.411 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0164 (generator column-GC/ECD, Miller et al. 1984,1985)
0.0202, 0.0193, 0.0232, 0.0266 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00708 (GC-RI correlation, Burkhard et al. 1985a)
0.0170 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0167, 0.0162 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00742 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 10.60 - 4440/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0123, 0.0182 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4229/(T/K) + 12.41$ (supercooled liquid P_L GC-RT correlation, Falconer & Bidleman 1994)
0.00955 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa m^3/mol at 25°C as indicated):
20.27 (calculated, Murphy et al. 1983)
47.72 (calculated-P/C, Burkhard et al. 1985b)
27.96 (20°C, calculated-P/C, Murphy et al. 1987)
37.90 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
21.28 (wetted-wall column-GC/ECD, Brunner et al. 1990)
35.79 (calculated-QSPR, Dunnivant et al. 1992)
22.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
39.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.23 (calculated-π constant, Bruggeman et al. 1982)
5.73 (generator column-GC/ECD, Miller et al. 1984, 1985)
6.22 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.86, 5.98, 5.77, 5.86 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.361 ± 0.046; 6.23 (slow stirring-GC, calculated-π const., De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.87 (recommended, Sangster 1993)
6.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.
8.57 (20°C, generator column-GC, measured range –10 to 20°C, Harner & Bidleman 1996)
9.64, 9.08, 8.57, 8.21 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Bidleman 1996)
$\log K_{OA} = -4.96 + 3981/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
9.08 (10°C, estimated, Thomas et al. 1998)
9.50, 8.63; 8.48 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.34 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
4.84; 6.37 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.84, 6.38 (zebrafish, kinetic approach: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
5.71 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.4 – 0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH\text{-}}(aq.) = 6.2 \times 10^9$ dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
$k_{OH}(calc) = (0.36 – 1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 3200\ d^{-1}$; $k_2 = 0.0458\ d^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.004\ d^{-1}$ with $t_{½}$ = 158 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½}$ = 196 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

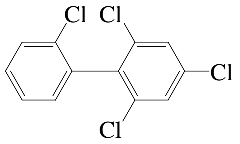
Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.25 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.99 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.31 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.39 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00094 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00243 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00168 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00147 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: depuration $t_{½}$ = 158 d for high-dose treatment, $t_{½}$ = 196 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.50 2,2′,4,6-Tetrachlorobiphenyl (PCB-50)



Common Name: 2,2′,4,6-Tetrachlorobiphenyl
Synonym: PCB-50, 2,2′,4,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,6-tetrachlorobiphenyl
CAS Registry No: 62796-65-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
45.0 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.092 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0320, 0.032, 0.030, 0.0412 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.1842 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.044 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C):
0.0451 (GC-RI correlation, Burkhard et al. 1985a)
0.0433 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
76.80 (gas stripping-GC, Atlas et al. 1982)
137.8 (calculated-P/C, Burkhard et al. 1985b)
58.57 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
61.76 (calculated-QSPR, Dunnivant et al. 1992)
28.68, 38.18, 49.84, 64.30 ± 1.4, 70.30 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 5.8937 - 2862.64/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(23.8/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.049/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R]$; where R = 8.314 $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
60.5 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 4$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.96 (calculated-TSA, Burkhard 1984)
5.72, 5.84, 5.70, 5.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.63 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.87 (calculated-MCI χ, Patil 1991)
5.75 (recommended, Sangster 1993)
5.6545 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

7.89 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.26, 3.50, 3.81 (algae, fish, activated sludge, Freitag et al. 1984,1985)

Sorption Partition Coefficient, log K_{OC}:

5.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4 – 0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

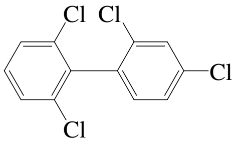
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.51 2,2′,4,6′-Tetrachlorobiphenyl (PCB-51)



Common Name: 2,2′,4,6′-Tetrachlorobiphenyl
Synonym: PCB-51
Chemical Name: 2,2′,4,6′-tetrachlorobiphenyl
CAS Registry No: 68194-04-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
66 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.396 (mp at 66°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0911 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.065 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.1842 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.044 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.033 (GC-RI correlation, Burkhard et al. 1985a)
0.0315 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
$\log (P/mmHg) = 10.40 - 4330/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0263 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4117/(T/K) + 12.20$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
76.80 (gas stripping-GC, Atlas et al. 1982)
101.2 (calculated-P/C, Burkhard et al. 1985b)
49.04 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
51.73 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.96 (calculated-TSA, Burkhard 1984)
5.86, 5.98, 5.77, 5.86 (RP-HPLC-k′ correlation, different stationary phases, Brodsky & Ballschmiter 1988)
5.63 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.88 (calculated-MCI χ, Patil 1991)
5.51 (recommended, Sangster 1993)
5.4591 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
7.62 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 10 food lipid (mg)/(g worm lipid-d); $k_{2:}$ = 0.11 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.006 d^{-1} with $t_{½}$ = 126 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 150 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

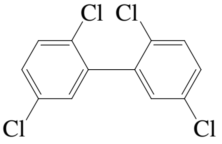
Sediment:

Soil:

Biota: elimination $t_{½}$ = 6 d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{½}$ = 126 d for high-dose treatment, $t_{½}$ = 150 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.52 2,2′,5,5′-Tetrachlorobiphenyl (PCB-52)



Common Name: 2,2′,5,5′-Tetrachlorobiphenyl
Synonym: PCB-52
Chemical Name: 2,2′,5,5′-tetrachlorobiphenyl
CAS Registry No: 35693-99-3
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
87–89 (Webb & McCall 1972; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point,)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
46.02 (Hinckley et al. 1990)
46.1 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.243 (calculated, assuming ΔS_{fus} = 56 J/mol K, Mackay et al. 1980)
0.316 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.046 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.0265 (shake flask-GC/ECD, Haque & Schmedding 1975)
0.016 (shake flask-LSC, Metcalf et al. 1975)
0.0060 (16.5°C, shake flask-GC/ECD, Wiese & Griffin 1978)
0.0223 (shake flask-GC/ECD from Aroclor 1242 mixture, Lee et al. 1979)
0.055 (generator column-GC/ECD, Bruggeman et al. 1981)
0.0365 (generator column-HPLC/UV, Huang 1983)
0.027 (generator column-GC/ECD, Miller et al. 1984; 1985)
0.0237, 0.0279, 0.0335, 0.0335 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.170 (generator column-HPLC/UV, Billington et al. 1988)
0.110; 0.461 (generator column-GC; supercooled liquid S_L, calculated-mp, Dunnivant & Elzerman 1988)
0.0153 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
0.0161 (shake flask-LSC, Eadie et al. 1990)
$\log (S_L/(\text{mol/L})) = -0.790 - 3352/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
0.0923 (calculated-mp and K_{OW}, Ran et al. 2002)
0.199, 0.140 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -1103/(T/K) + 0.37$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00733 (solid P_S from GC-RT correlation, Westcott & Bidleman 1981)
0.00253, 0.0048(solid P_S, 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
$\log (P_S/\text{mmHg}) = 11.8 - 4920/(T/K)$, temp range 30–40°C (gas saturation-GC, Westcott et al. 1981)
0.104; 0.428(solid P_S; supercooled liq. P_L calculated from P_S using fugacity ratio F, Neely 1981)
0.0188, 0.0165(P_{GC} by GC-RT correlation, different GC stationary phases, Bidleman 1984)

0.0104 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
0.0159, 0.0229(supercooled liquid P_L calculated from P_{GC}, GC-RT correlation, different stationary phases, Bidleman 1984)
0.00492 (GC-RI correlation, Burkhard et al. 1985a)
0.00497; 0.0193(selected exptl. P_S; supercooled liquid P_L, GC-RI correlation, Burkhard et al.1985)
0.0184, 0.0173(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0049; 0.0020(selected solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
0.00904 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0127; 0.0546(calculated-S × HLC; solid P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
log (P/mmHg) = 10.60 – 4430/(T/K) (GC-RT correlation, supercooled liquid, Tateya et al. 1988)
0.0104, 0.008(supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.0188, 0.012 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (P_L/Pa) = 11.74 – 4127/(T/K) (GC-RT correlation, Hinckley et al. 1990)
0.0132, 0.020 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4220/(T/K) + 12.36 (supercooled liq. P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.00690; 0.00218 (solid P_S; supercooled liq. P_L, Passivirta et al. 1999)
log (P_S/Pa) = 14.77 – 5087/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 12.36 – 4220/(T/K) (liquid, Passivirta et al. 1999)
0.0033–0.013; 0.00901–0.0512 (literature P_S range; literature P_L range, Delle Site 1997)
0.00904 (supercooled liquid P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.0107, 0.0120 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log (P_L/Pa) = –4190/(T/K) + 12.08 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log (P_L/Pa) = –4059/(T/K) + 11.69 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
31.41–53.7 (calculated-P/C, Westcott et al. 1981)
14.1–53.7 (calculated-P/C, Westcott & Bidleman 1981)
94.15 (gas stripping-GC/ECD, Atlas et al. 1982)
22.29 (calculated-P/C, Murphy et al. 1983)
26.34 (calculated-P/C, Murphy 1984)
31.41–53.70 (calculated-P/C, Bidleman 1984)
53.20 (calculated-P/C, Burkhard et al. 1985b)
2.53 (batch stripping-GC, Hassett & Milicic 1985)
12.16 (20°C, gas stripping-GC, Oliver 1985)
47.59 (calculated-P/C, Shiu & Mackay 1986)
24.11 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
34.65 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988)
44.04 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
32.34 (calculated-QSPR, Dunnivant et al. 1992)
16.4* (20°C, gas stripping-HPLC/fluorescence, measured range 10–48°C, ten Hulscher et al. 1992)
17.0 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
28.78 ± 3.4 (gas stripping-GC/ECD, Girvin et al. 1997)
log [H/(Pa m^3/mol)] = 13.15 – 3552/(T/K) (Passivirta et al. 1999)
31.07* ± 0.42 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$K_{AW} = \exp[-(30.5/\text{kJ·mol}^{-1})/RT] + (0.066/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
28.27 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 2001)
log K_{AW} = 6.427 – 2530/(T/K) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
31.3 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 31 ± 3 kJ/mol, ΔS_H = 0.07 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
28.18, 25.12 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

log [H/(Pa m^3/mol)] = –2189/(T/K) + 8.79 (LDV linear regression of literature data, Li et al. 2003)
log [H/(Pa m^3/mol)] = –2956/(T/K) + 11.32 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
3.91 (shake flask-radiolabeled-^{14}C-LSC, Metcalf et al. 1975)
5.81 (Hansch & Leo 1979)
6.26 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.09 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.81, 5.87, 5.43, 5,80 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.02 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
5.81 (generator column-GC, Larsen et al. 1992)
6.00 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.79 (recommended, Sangster 1993)
6.09 (recommended, Hansch et al. 1995)
6.10 (calculated, Passivirta et al. 1999)
6.00, 5.91 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:
7.90 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
8.22; 7.73 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = –6.20 + 4340/(T/K); temp range: 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
9.10 (10°C, estimated, Thomas et al. 1998)
9.46, 8.49; 8.56 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.33 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.47; 8.44 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.22, 8.22 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4251/(T/K) – 6.04 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
3.87 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)
4.26, 4.60, 4.02, 4.07 (algae, snail, mosquito, fish, Metcalf et al. 1975)
2.66 (green sunfish, 15 d in static water, Sanborn et al. 1975)
6.21; 6.07 (goldfish, 3% lipid; 10% lipid dry wet in food, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
6.38 (guppy, 3.5% lipid, Bruggeman et al. 1982,1984; quoted, Gobas et al. 1987)
4.69, 4.98 (goldfish, exptl., correlated, Mackay & Hughes 1984)
3.49–4.26 highest value 4.26, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
5.30, 4.26; 6.28(rainbow trout, laboratory data: kinetic BCF (k_1/k_2), steady state BCF (C_F/C_W); Lake Ontario field BCF, Oliver & Niimi 1985)
4.26, 4.69 (guppy, goldfish, calculated-C_B/C_W, or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
4.26 (fish, quoted, Isnard & Lambert 1988,1989)
6.38; 5.76 (guppy, lipid wt. based, corrected lipid wt. based, Gobas et al. 1989)
4.25 (guppy, estimated, Banerjee & Baughman 1991)
6.21; 6.32 (lipid basis: goldfish; rainbow trout, Noegrahati & Hammers 1992)
4.54, 6.02; 4.782, 4.708 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
3.08–4.58 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.86–6.31 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.23 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
5.03, 4.67; 3.57, 4.76, 4.17, 5.39 (oligochaetes; chironomid larvae, Bott & Standley 2000)
3.36, 5.60 (*Daphnia*, 21-d renewal: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.87, 6.12 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)

4.28, 6.23 (mussel *Mutilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.42, 6.34 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.63, 5.93 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.69, 5.99 (goldfish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.92, 6.46 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.01; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Bioaccumulation Factor, log BAF at 25°C or as indicated:

7.38 (rainbow trout, lipid based-L/kg(Ip), quoted, Thomann 1989)
4.92; 6.43 (22°C, zebrafish: log BCF$_W$ wet wt basis; log BCF$_L$ lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.60, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.73–5.15 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

4.67 (Woodburn soil silt loam, sorption isotherm measurement, Haque & Schmedding 1976)
5.91 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.60; 5.50; 5.70 (field data of sediment trap material; Niagara River-organic matter; calculated-K_{OW}, Oliver & Charlton 1984)
4.54, 4.42 (Aldrich humic acid with 9.4 mg/L DOC: reversed-phase separation, equilibrium dialysis, Landrum et al. 1984)
3.87, 4.36 (Huron River water with 7.8 mg/L DOC: reversed-phase separation, equilibrium dialysis, Landrum et al. 1984)
4.87 (dissolved humic acid, gas purging-LSC, Hassett & Milicic 1985)
5.35 (suspended solids-Lake Superior; field measurement-GC/ECD, Baker et al. 1986)
5.70, 4.87 (Lake Superior suspended solids: calculated-KOW, Baker et al. 1986)
6.15 (Composite Condie silt soil 0.36% OC, batch sorption equilibrium, Anderson & Pankow 1986)
5.0–6.4, 5.9 (suspended sediment, range, average, Oliver 1987a)
6.12 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.65 (calculated, Bahnick & Doucette 1988)
3.48 (12 lakes/streams in southern Ontario at 1.6–26.5 mg/L DOC, Evans 1988)
4.35 (calculated-polymaleic acid, Chin & Weber 1989)
5.88 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.88 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.83 (organic carbon from total suspended matter of raw water from Lake Michigan, Eadie et al. 1990)
5.00, 3.88 (Aldrich humic acid, natural DOC, reversed-phase separation, Eadie et al. 1990)
5.00; 4.38–4.81; 2.89–3.93 (Aldrich humic acid; humic acid from soil & water samples; fulvic acid & dissolved organic matter samples, Jota & Hassett 1991)
6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.41 (soil, batch sorption equilibration-GC, Paya-Perez et al. 1991)
6.04, 4.80 (Hamlet City lake sediment, WES reference soil, batch sorption equilibrium, Brannon et al. 1995)
4.73 (Ispra oil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
5.02, 6.04; 4.80 (sediments from Brown's Lake, Hamlet City Lake; WES reference soil, shake flask-HPLC/fluorescence, Brannon et al. 1995)
4.97; 5.09 (soil, quoted lit.; calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.30–5.41 (soil-Catlin silt loam, f_{OC} = 0.0226, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.61–5.65 (Cloudland loam, f_{OC} = 0.0024, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997
5.30–5.31 (Kenoma silt loam, f_{OC} = 0.0153, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.38 (Kenoma silt loam, f_{OC} = 0.0092, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.43–5.53 (Kenoma silt loam, f_{OC} = 0.002, depth 120–155 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.26–5.44 (Norborne silt loam, f_{OC} = 0.0137, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)

5.24–5.36 (Norborne silt loam, f_{OC} = 0.009, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.39–5.40 (Norborne silt loam, f_{OC} = 0.0057, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)
5.50; 4.90 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
4.98 (sediment, Bott & Standley 2000)
5.02, 4.55 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
5.58 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)
3.79–6.07; 4.40–6.40(range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.32; 5.52, 5.38, 5.60(20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log K_{OM}:
4.67 (Haque & Schmedding 1976; Chou & Griffin 1986)
4.67, 4.62 (quoted, calculated-MCI χ, Sabljic 1984)
3.88 (Great Lake DOC, reversed-phase separation, Eadie et al. 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: $t_{½}$(exptl) = 2.8 h of evaporation from an initial concentration of 0.005 ppm in a glass dish of 4.5 cm depth of water solution at 24°C and $t_{½}$ = 0.68 h with stirring of the solution (Chiou et al. 1979); depletion k = 34 d^{-1} from a 26-cm or 67-cm height purge vessels. from aqueous solution (Girvin et al. 1997).
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation: microbial degradation with pseudo first-order rate constant k = 0.1 yr^{-1} in the water column and k = 1.0 yr^{-1} in the sediment (Furukawa et al. 1978; quoted, Neely 1981).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.008 d^{-1} (11°C, rainbow trout, Guiney et al. 1977; quoted, Waid 1986)
k_2 = 0.003 d^{-1} (10–11°C, rainbow trout eggs and sac fry, Guiney et al. 1980; quoted, Waid 1986)
k_1 = 740 d^{-1}; k_2 = 0.015 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986; Clark et al. 1990)
k_1 = 280 d^{-1}; k_2 = 0.0014 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_1 = 1200 d^{-1}; k_2 = 0.015 d^{-1} (guppy, Bruggeman et al. 1984)
k_2 = 0.015, 0.0134 d^{-1} (goldfish, exptl., correlated, Mackay & Hughes 1984)
k_1 = 2800 d^{-1}; k_2 = 0.0014 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_1 = 30.8 h^{-1}; $1/k_2$ = 1600 h (goldfish, quoted, Hawker & Connell 1985)
k_1 = 50.0 h^{-1}; $1/k_2$ = 1600 h (guppy, quoted, Hawker & Connell 1985)
k_1 = 1100 d^{-1} (guppy, Opperhuizen 1986)
log k_1 = 2.87 d^{-1}; log $1/k_2$ = 1.82 d (fish, quoted, Connell & Hawker 1988)
log $1/k_2$ = 2.9, 3.0 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b).
$1/k_2$ = 30.3 d (guppy, quoted, Clark et al. 1990)
$1/k_2$ = 61.7, 102 d (guppy, Gobas et al. 1989; quoted, Clark et al. 1990)
k_1 = 3230 d^{-1}; k_2 = 0.0387 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.011 d^{-1} with $t_{½}$ = 65 d and k_2 = 0.018 d^{-1} with $t_{½}$ = 39 d for food concn of 22 ng/g and 125 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_1 = 20 L d^{-1} g^{-1} dry wt.; k_2 = 0.118 d^{-1} (Baltic Sea blue mussels, flow-through experiment., Gustafsson et al. 1999)

$k_1 = 0.00061\ h^{-1}$; $k_2 = 0.0115\ h^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1(calc) = 9 (food lipid mg)/(g worm lipid-d); k_2(calc) = $0.09\ d^{-1}$ (earthworm, Wågman et al. 2001)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 158$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 196$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
$k_2 = 0.015\ d^{-1}$ with $t_{½} = 46.2$ d (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1996);
$t_{½}$ = 1500 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: $t_{½}$ = 19.7 d in Lake Michigan (Neely 1983);
$t_{½}$ = 30000 h at 7°C for Baltic Proper environment (estimated, Sinkkonem & Passivirta 2000).
Groundwater:
Sediment: $t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.27\ d^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.99\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.30\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.39\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00112\ d^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00251\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00174\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00127\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).
$t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: $t_{½}$ = 1.76 yr in female rainbow trouts, $t_{½}$ = 1.43 yr in males (Guiney et al. 1980);
$t_{½}$ = 500 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985); and $t_{½}$ = 99 d in its muscle, (Niimi & Oliver 1983);
$t_{½}$ = 46 d in guppy (Bruggeman et al. 1984);
$t_{½}$ = 43 d in worms at 8°C, 43 d (Oliver 1987c)
depuration $t_{½}$ = 39–65 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
theoretical half-life to reach 90% steady-state tissue concn 5.9 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);
$t_{½}$ = 6.0 h in blood plasma (ring doves, Drouillard & Norstrom 2000)
elimination $t_{½}$ = 8 d in earthworm given contaminated food (predicted, Wågman et al. 2001).
depuration $t_{½}$ = 158 d for high-dose treatment, $t_{½}$ = 196 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
depuration $t_{½}$ = 46.2 d for juvenile carp in 100-d experiment (Stapleton et al. 2004)

TABLE 7.1.1.52.1

Reported vapor pressures and Henry's law constants of 2,2′,5,5′-tetrachlorobiphenyl (PCB-52) at various temperatures and temperature dependence equations

Vapor pressure		Henry's law constant			
Westcott et al. 1981		ten Hulscher et al. 1992		Bamford et al. 2000	
gas saturation-GC/ECD		gas stripping-GC		gas stripping-GC/MS	
t/°C	P/Pa	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
25	0.00253	10.4	8.6	4	11.34
30	0.0048	20.0	16.4	11	16.13
		30.1	37.4	18	22.56
		34.9	38.8	25	31.07
log P = A – B/(T/K)		42.1	68.7	31	40.43
	P/mmHg	47.9	109.2		
A	11.8	48.4	120.6		
B	4920			$\ln K_{AW} = -\Delta H/RT + \Delta S/R$	
temp range 30–40°C		$\ln K_{AW} = A - B/(T/K)$		A	7.9384
		A	23.387	B	3668.5
		B	6254.5		
				enthalpy, entropy change:	
		enthalpy of volatilization:		$\Delta H/(kJ \cdot mol^{-1}) = 30.5 \pm 2.8$	
		$\Delta H_{vol}/(kJ \cdot mol^{-1}) = 52.0 \pm 5$		$\Delta S/(J \cdot K^{-1}\ mol^{-1}) = 66 \pm 10$	
		entropy of volatilization, ΔS:			
		$T\Delta S_{vol}/(kJ \cdot mol^{-1}) = 57.0 \pm 6$			
		at 20°C			

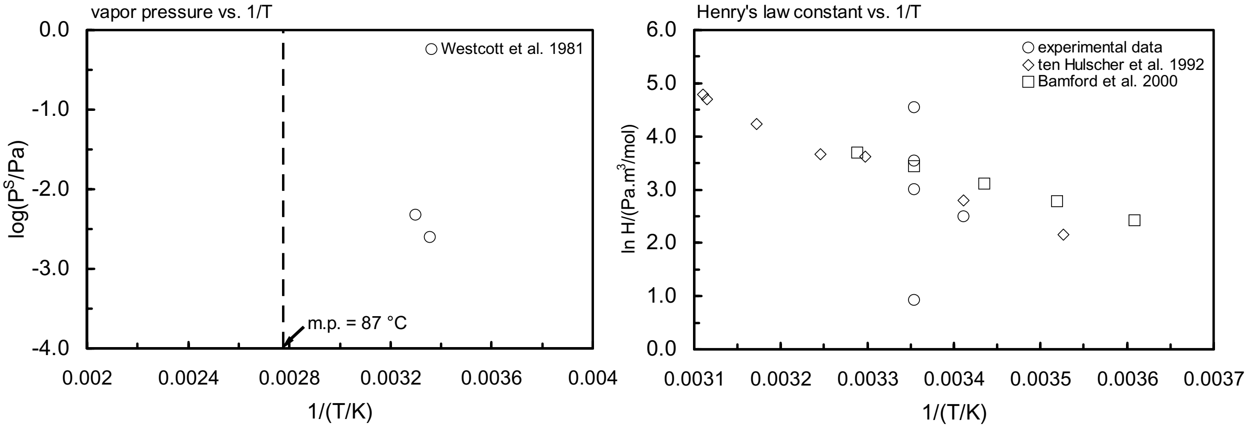
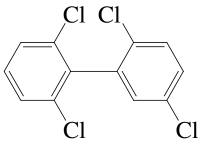


FIGURE 7.1.1.52.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for 2,2′,5,5′-tetrachlorobiphenyl (PCB-52).

7.1.1.53 2,2′,5,6′-Tetrachlorobiphenyl (PCB-53)



Common Name: 2,2′,5,6′-Tetrachlorobiphenyl
Synonym: PCB-53, 2,2′,5,6′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,5,6′-tetrachlorobiphenyl
CAS Registry No: 41464-41-9
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
 103–104.5 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
 268.2 (calculated-Le Bas method at normal boiling point)
 211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.168 (mp at 104°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
 0.0923 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
 0.109 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
 0.0945, 0.0786, 0.0717, 0.0335 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 0.0476 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
 0.288 (supercooled liquid S_L, calculated-mp, Dunnivant & Elzerman 1988)
 0.292 (calculated-TSA, Abramowitz & Yalkowsky 1990)
 0.044 (calculated-MCI χ, Patil 1991)
 0.0520 (calculated-QSPR, Dunnivant et al. 1992)
 0.0306 (calculated-group contribution, Kühne et al. 1995)
 0.0114, 0.0306 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
 0.114 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 0.00493 (Neely 1983; quoted, Erickson 1986)
 0.0273 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
 0.0356 (supercooled liquid P_L, GC-RT correlation, Burkhard 1984)
 0.0372 (GC-RI correlation, Burkhard et al. 1985a)
 0.0356 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
 0.0268, 0.0331 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 0.011 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
 0.00671; 0.0405 (calculated-S × HLC, solid P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
 $\log (P/\text{mmHg}) = 10.40 - 4310/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
 0.0214, 0.0347 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/)a) = -4114/(T/K) + 12.24$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
 0.0162 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994. Harner & Bidleman 1996)
 0.00161–0.0204; 0.0107–0.0385 (literature P_S range; literature P_L range, Delle Site 1997)
 0.00955 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], reported as 2,2′,5,6- Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C as indicated):

30.40 (calculated-P/C, Murphy et al. 1983)
112.5 (calculated-P/C, Burkhard et al. 1985b)
28.67 (20°C, calculated-P/C, Murphy et al. 1987)
41.14 (batch stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
47.26 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
43.62 (calculated-QSPR, Dunnivant et al. 1992)
17.21 (calculated-QSPR, Achman et al. 1993)
44.8 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.96 (calculated-TSA, Burkhard 1984)
5.90 (calculated-regression analysis with chlorine substituents, Oliver 1987c)
5.39, 5.57, 5,43, 5.80 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.46 (generator column-GC, Hawker & Connell 1988a)
5.62 (calculated-TSA, Hawker & Connell 1988a)
5.87 (calculated-MCI χ, Patil 1991)
5.55 (recommended, Sangster 1993)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
5.98 (quoted, Hansch et al. 1995)
6.12, 5.55–5.90 (calculated-Characteristic Root Index CRI, min.-max. range, Saçan & Inel 1995)
5.4429 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.13 (calculated-CLOGP ver. 4, Ran et al. 2002)
5.67 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

9.28, 8.70, 8.24, 7.64 (0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
$\log K_{OA} = -5.26 + 3965/(T/K)$; temp range 0–30°C (generator column-GC, Harner & Bidleman 1996)
9.18, 8.18; 8.25 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 5.7 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation: 91% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0019\ d^{-1}$ (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

$k_2 = 0.008\ d^{-1}$ with $t_{1/2} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008\ d^{-1}$ with $t_{1/2} = 88$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

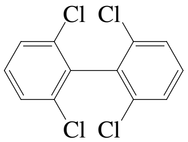
Soil:

Biota: $t_{1/2} = 365$ d in rainbow trout, d and $t_{1/2} = 107$ d in its muscle 107 d (Niimi & Oliver 1983);

$t_{1/2} = 30$ d in worms at 8°C, 30 d (Oliver 1987c).

depuration $t_{1/2} = 91$ d for high-dose treatment, $t_{1/2} = 88$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.54 2,2′,6,6′-Tetrachlorobiphenyl (PCB-54)



Common Name: 2,2′,6,6′-Tetrachlorobiphenyl
Synonym: PCB-54, 2,2′,6,6′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,6,6′-tetrachlorobiphenyl
CAS Registry No: 15968-05-5
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
198 (Van Roosmalen 1934; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0201 (mp at 198°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.412, 0.221, 0.143, 0.0882 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0027 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
0.0119 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0659 (supercooled liquid P_L, Burkhard 1984)
0.00132 (GC-RI correlation, Burkhard et al. 1985a)
0.0659 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0392, 0.0517 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0566 (supercooled liquid P_L, Dunnivant & Elzerman 1988)
0.00227; 0.118 (calculated-S × HLC, P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
$\log (P_L/Pa) = -3751/(T/K) + 11.17$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.000396–0.0219; 0.00388–0.104 (literature P_S range; literature P_L range, Delle Site 1997)
0.0114 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C):
188.5 (calculated-P/C, Burkhard et al. 1985b)
15.0 (calculated, Coates & Elzerman 1986)
55.73 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
50.0 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
50.04 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.63 (calculated after Rekker 1977, Könemann 1981)
4.16, 713, 7.01 (HPLC-k′ correlation; calculated-π const.; calculated-fragment const., McDuffie 1981)

5.94 (RP-TLC-retention, Bruggeman et al. 1982)
4.95, 5.27, 5.22, 5.52 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.48 (generator column-GC, Hawker & Connell 1988a)
5.936 ± 0.031 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.24 (recommended, Sangster 1993)
5.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
7.30 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

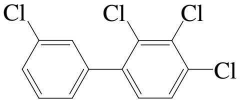
Bioconcentration Factor, log BCF:
3.85; 5.38 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:
5.106, 4.91, 4.89, 4.72 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
5.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.63 (river sediment, Coates & Elzerman 1986)
4.79 (correlated literature values in soils, Sklarew & Girvin 1987)
5.01 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
5.11; 5.01 (soil, quoted lit.; calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
4.91, 4.84 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.4 – 0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:
k_1 = 2740 d^{-1}; k_2 = 0.387 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{1/2}$ = 190 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.007 d^{-1} with $t_{1/2}$ = 100 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: photodegradation $t_{1/2}$ = 72.5 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5 kW high pressure Xenon lamp (De Felip et al. 1996).
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{1/2}$ = 190 d for high-dose treatment, $t_{1/2}$ = 100 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.55 2,3,3′,4-Tetrachlorobiphenyl (PCB-55)



Common Name: 2,3,3′,4-Tetrachlorobiphenyl
Synonym: PCB-55, 2,3,3′,4-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4-tetrachlorobiphenyl
CAS Registry No: 74338-24-2
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
89 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.122 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.81×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00517 (GC-RI correlation, Burkhard et al. 1985b)
0.00579, 0.00349 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4382/(T/K) + 12.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
11.55 (calculated-P/C, Burkhard 1984)
23.51 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
18.48 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 2$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.86 (calculated-TSA, Burkhard 1984)
6.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0161 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.66 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Live, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.008$ d^{-1} with $t_{½} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d^{-1} with $t_{½} = 157$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

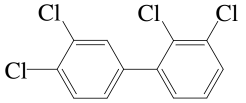
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½} = 91$ d for high-dose treatment, $t_{½} = 157$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.56 2,3,3′,4′-Tetrachlorobiphenyl (PCB-56)



Common Name: 2,3,3′,4′-Tetrachlorobiphenyl
Synonym: PCB-56, 2,3,3′,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′-tetrachlorobiphenyl
CAS Registry No: 41464-41-9
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
95 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.122 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0389 (20°C, supercooled liquid, Murphy et al. 1987)
0.0989 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0146 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0115 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.96×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00517 (GC-RI correlation, Burkhard et al. 1985b)
0.00434, 0.00327 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.17×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.00331, 0.00468 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4382/(T/\text{K}) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
9.45 (calculated-P/C, Burkhard 1984)
16.41 (20°C, calculated-P/C, Murphy et al. 1987)
13.27 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
15.34 (calculated-QSAR, Dunnivant et al. 1992)
8.24 (calculated-QSAR, Achman et al. 1993)
13.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
27.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 32 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.86 (calculated-TSA, Burkhard 1984)
5.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.11 (calculated, Miertus & Jakus 1990)
5.85 (recommended, Sangster 1993)

5.90 (calculated-TSA, Murray & Andren 1992)
5.9815 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

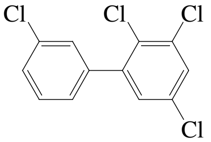
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.66 (suspended particulate matter, Burkhard 1984)
6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH\cdot}$(aq.) = 5.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota:

7.1.1.57 2,3,3′,5-Tetrachlorobiphenyl (PCB-57)



Common Name: 2,3,3′,5-Tetrachlorobiphenyl
Synonym: PCB-57
Chemical Name: 2,3,3′,5-tetrachlorobiphenyl
CAS Registry No: 70424-87-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 291.988
Melting Point (°C):
68 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0718 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00767 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
19.76 (calculated-P/C, Burkhard 1984)
37.59 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
27.40 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated, Burkhard 1984)
6.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.1376 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.69 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

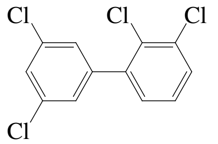
Ground water:

Sediment:

Soil:

Biota:

7.1.1.58 2,3,3′,5′-Tetrachlorobiphenyl (PCB-58)



Common Name: 2,3,3′,5′-Tetrachlorobiphenyl
Synonym: PCB-58
Chemical Name: 2,3,3′,5′-tetrachlorobiphenyl
CAS Registry No: 41464-43-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
68 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00558 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
9.62×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000167 (GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 10.80 – 5600/(T/K) (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C or as indicated):
16.11 (calculated-P/C, Burkhard 1984)
45.46 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
25.33 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.17 (calculated-TSA, Hawker & Connell 1988a)
6.17 (recommended, Hansch et al. 1995)
6.0904 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.73 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

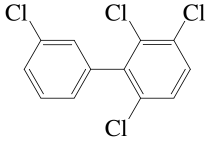
Ground water:

Sediment:

Soil:

Biota:

7.1.1.59 2,3,3′,6-Tetrachlorobiphenyl (PCB-59)



Common Name: 2,3,3′,6-Tetrachlorobiphenyl
Synonym: PCB-59
Chemical Name: 2,3,3′,6-tetrachlorobiphenyl
CAS Registry No: 74472-33-6
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.131 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00733 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0155 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0164 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
34.65 (calculated-P/C, Burkhard 1984)
36.58 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
30.81 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated, Burkhard 1984)
5.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8476 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.64 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.005 d^{-1} with $t_{½}$ = 132 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 135 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

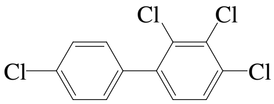
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 132 d for high-dose treatment, $t_{½}$ = 135 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.60 2,3,4,4′-Tetrachlorobiphenyl (PCB-60)



Common Name: 2,3,4,4′-Tetrachlorobiphenyl
Synonym: PCB-60, 2,3,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′-tetrachlorobiphenyl
CAS Registry No: 33025-41-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
  128 (Weast 1972–73; Ruelle & Kesselring 1997)
  142 (Saeki et al. 1971; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
  268.2 (calculated-Le Bas method at normal boiling point)
  211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.0695 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.058 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
  0.0168 (calculated-TSA, Mackay et al. 1980)
  0.121 (calculated-TSA, supercooled liquid S_L, Burkhard et al. 1985b)
  0.0389 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  0.0902, 0.0485, 0.0254, 0.0243 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  0.0359, 0.0273 (Nirmalakhandan & Speece 1989)
  0.0146 (calculated-TSA, Abramowitz & Yalkowsky 1990)
  0.045 (calculated-MCI χ, Patil 1991)
  0.00274 (calculated-QSPR, Dunnivant et al. 1992)
  0.0067, 0.0176 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.000319 (GC-RI correlation, Burkhard et al. 1985a)
  0.00427 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  0.00527, 0.00414 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.00217 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  log (P/mmHg) = 10.90 – 4660/(T/K) (GC-RT correlation, Tateya et al. 1988)
  0.00331, 0.00458 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
  log (P_L/Pa) = – 4282/(T/K) + 12.42 (supercooled liquid P_L, GC-RT correlation, Falconer Bidleman 1994)
  0.0157 (supercooled liquid P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C):
  84.20 (batch stripping, Atlas et al. 1982)
  10.34 (calculated-P/C, Burkhard et al. 1985b)
  16.41 (20°C, calculated-P/C, Murphy et al. 1987)

15.40 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
15.48 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.87 (calculated-TSA, Burkhard 1984)
5.84 (HPLC-RT correlation calculated-π, Rapaport & Eisenreich 1984)
5.90 (selected, Shiu & Mackay 1986)
5.89, 6.15, 6.57, 6.37 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.11 (calculated-TSA, Hawker & Connell 1988a)
5.88 (calculated-MCI χ, Patil 1991)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.01 (recommended, Sangster 1993)
5.84 (quoted, Hansch et al. 1995)
5.95, 5.33–6.24 (calculated-Characteristic Root Index CRI, minimum-maximum range, Saçan & Inel 1995)
6.0108 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.82 (10°C, estimated, Thomas et al. 1998)
9.21 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
6.20, 5.0 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
5.67 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.10 (organic carbon, obs., Murray & Andren 1992)
5.03 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.30 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH\cdot}$(aq.) = 5.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 10 (food lipid mg)/(g worm lipid-d); k_2 = 0.10 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

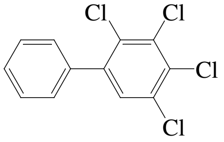
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 7 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.61 2,3,4,5-Tetrachlorobiphenyl (PCB-61)



Common Name: 2,3,4,5-Tetrachlorobiphenyl
Synonym: PCB-61, 2,3,4,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4,5-tetrachlorobiphenyl
CAS Registry No: 33284-53-6
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
92.2 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
25.2 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
69.45 (Miller et al. 1984)
69.25, 64.3 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.217 (Mackay et al. 1980)
0.218 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0192 (generator column-GC/ECD, Weil et al. 1974)
0.0209 (shake flask-GC/ECD, Haque & Schmedding 1975)
0.0099 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)
0.0209 (generator column-GC/ECD, Miller et al. 1984, 1985)
0.0207, 0.030, 0.0180, 0.0243 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.014 (generator column-GC, Dunnivant & Elzerman 1988)
0.0137 (generator column-GC/ECD, Li et al. 1992; Li & Doucette 1993)
0.0136 (shake flask-GC/ECD, Li & Andren 1994)
0.0156* ± 0.0004 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
$\ln x = -3.967 - 4970.5/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0624 (calculated-mp and K_{OW}, Ran et al. 2002)
0.106, 0.101 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log [S_L/(mol\ m^{-3})] = -839/(T/K) - 0.626$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log [S_L/(mol\ m^{-3})] = -1043/(T/K) + 0.037$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0013 (GC-RT correlation, Burkhard et al. 1985a)
0.00558 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
$\log (P_L/Pa) = -4382/(T/K) + 12.78$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
1.854×10^{-4}* (20°C, gas saturation-GC/ECD, measured range –20 to 20°C, Wania et al. 1994)
$\log (P_S/Pa) = 12.10 - 4632/(T/K)$; temp range –20 to + 20°C (gas saturation-GC, Wania et al. 1994)

0.0144 (supercooled liq. P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.00724, 0.00692 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log (P_L/Pa) = -4330/(T/K) + 12.38$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log (P_L/Pa) = -4193/(T/K) + 11.91$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
11.45 (calculated-P/C, Burkhard et al. 1985b)
17.53 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
24.14 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
20.42, 19.95 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -3150/(T/K) + 11.87$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
5.78 (HPLC-RT correlation, Sugiura et al. 1979)
5.90 (shake flask-GC, Platford 1982)
6.39 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.74 (calculated-fragment const., Yalkowsky et al. 1983)
5.81 (calculated-TSA, Burkhard 1984)
5.72 (generator column-GC/ECD, Miller et al. 1984,1985)
5.90 (selected, Shiu & Mackay 1986)
6.38, 6.31, 6.57, 6.37 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.18; 6.04 (generator column-GC/ECD; calculated-TSA, Hawker & Connell 1988a)
5.92, 6.74 (calculated-solvatochromic parameters and V_I, calculated- fragment additivity., Kamlet et al. 1988)
6.88, 6.74, 5.89, 6.04, 6.02 (calculated-π const., f const., MW, MCI χ, TSA, Doucette & Andren 1988)
6.39 (calculated-π const., De Bruijn et al. 1989)
6.406 ± 0.069 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.89 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.34 (generator column-GC, Li & Doucette 1993)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.44 (recommended, Sangster 1993)
6.41 (recommended, Hansch et al. 1995)
5.97, 5.72–6.74 (calculated-Characteristic Root Index CRI; minimum-maximum range, Saçan & Inel 1995)
6.1472 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.00 (calculated-QSPR, Yeh & Hong 2002)
6.51 (calculated-CLOGP ver. 4, Ran et al. 2002)
6.17, 6.11 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
8.901* (20°C, generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)
$\log K_{OA} = -2.90 + 3464/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Mackay 1995)
8.90 (20°C, generator column-GC, Harner & Bidleman 1996)
$\log K_{OA} = -2.89 + 3464.1/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
9.38–9.65 (10°C, estimated, Thomas et al. 1998)
10.19, 8.93; 8.90 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.76 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.80; 8.75 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.64, 8.55 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4660/(T/K) - 7.08$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
4.29, 3.57, 3.94, 3.90 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

Sorption Partition Coefficient, log K_{OC}:

5.61 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.93 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.038\ d^{-1}$ (golden orfe, Sugiura et al. 1979)
$k_2 = 0.0022\ d^{-1}$ (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 312 d in rainbow trout, and $t_{½}$ = 93 d in its muscle 93 d (Niimi & Oliver 1983)

TABLE 7.1.1.61.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,3,4,5-tetrachlorobiphenyl (PCB-61) at various temperatures

Aqueous solubility		**Vapor pressure**		**log K_{OA}**	
Shiu et al. 1997		**Wania et al. 1994**		**Harner & Mackay 1995**	
generator column-GC/ECD		**gas saturation-GC/ECD**		**generator column-GC**	
t/°C	**$S/g \cdot m^{-3}$**	**t/°C**	**P/Pa**	**t/°C**	**log K_{OA}**
5	0.0056	–20	5.298×10^{-7}	–10	10.268
15	0.0102	–10	3.817×10^{-6}	0	9.80
25	0.0156	0	1.439×10^{-5}	10	9.40
35	0.0285	10	6.163×10^{-5}	20	8.901
45	0.0560	20	1.854×10^{-4}	25	8.74
		log (P/Pa) = A – B/(T/K)		ΔH_{OA}/(kJ mol⁻¹) = 66.3	
ΔH_{sol}/(kJ mol⁻¹) = 41.3		A	12.10		
	for 5–45°C	B	4632	log K_{OA} = A + B/T	
		temp range –20 to20°C		A	–2.9
				B	3464.1
		ΔH_{subl}/(kJ mol⁻¹) = 88.7			

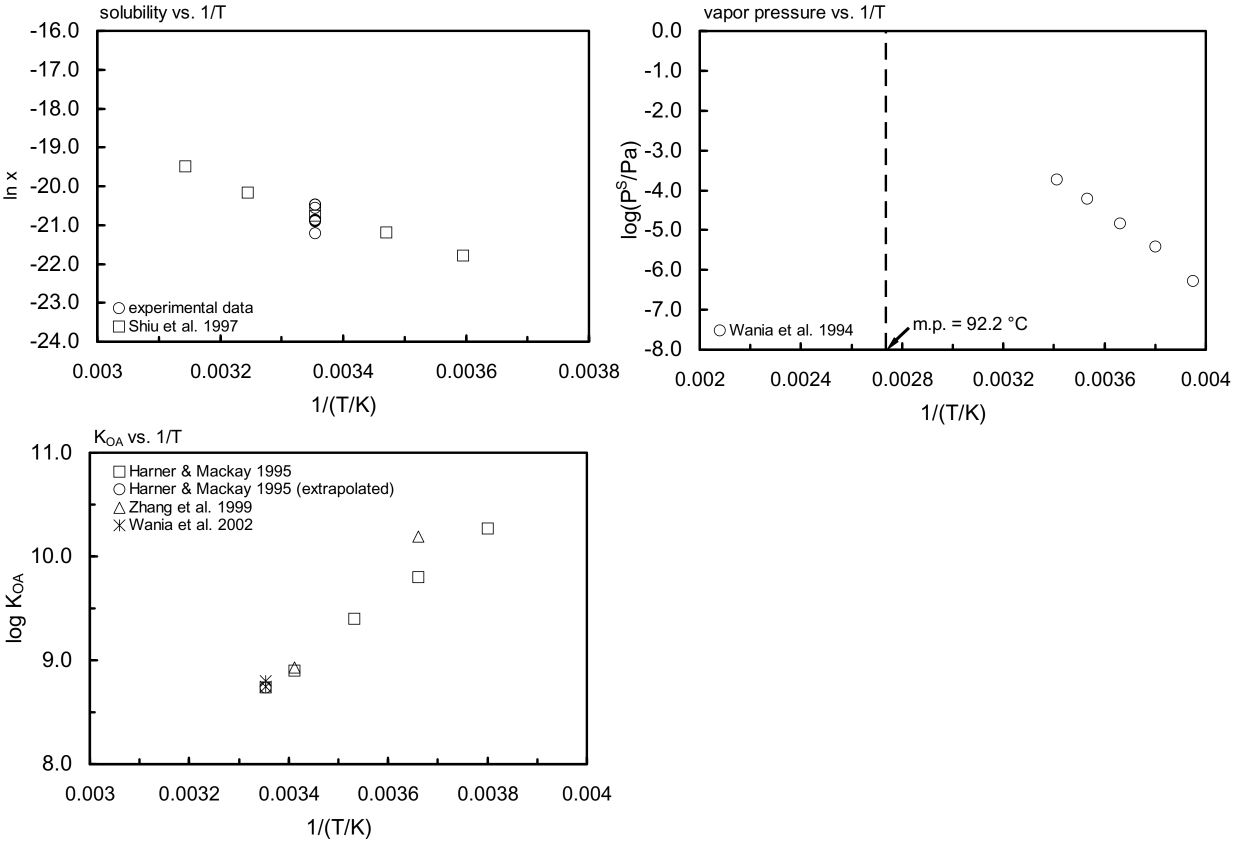
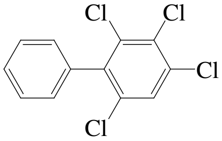


FIGURE 7.1.1.61.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,3,4,5-tetrachlorobiphenyl (PCB-61).

7.1.1.62 2,3,4,6-Tetrachlorobiphenyl (PCB-62)



Common Name: 2,3,4,6-Tetrachlorobiphenyl
Synonym: PCB-62
Chemical Name: 2,3,4,6-tetrachlorobiphenyl
CAS Registry No: 54230-23-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):

77	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

268.2	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.151	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0463	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):

0.0158	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0167	(GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

30.70	(calculated-P/C, Burkhard 1984)
37.08	(calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
21.28	(wetted-wall column-GC, Brunner et al. 1990)
37.47	(calculated-QSPR, Dunnivant et al. 1992)
35.0	(predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.79	(calculated, Burkhard 1984)
5.89	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0323	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

8.81	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.59	(suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

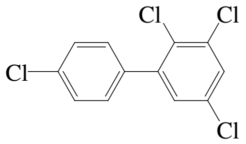
Ground water:

Sediment:

Soil:

Biota:

7.1.1.63 2,3,4′,5-Tetrachlorobiphenyl (PCB-63)



Common Name: 2,3,4′,5-Tetrachlorobiphenyl
Synonym: PCB-63, 2,3,4′,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4′,5-tetrachlorobiphenyl
CAS Registry No: 74472-34-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
83 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.105 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0263 (20°C, supercooled liquid, Murphy et al. 1987)
0.0496 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00727 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.36×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00681 (GC-RI correlation, Burkhard et al. 1985b)
2.64×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.00724 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4382/(T/K) + 12.53$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
17.73 (calculated-P/C, Burkhard 1984)
29.28 (20°C, calculated-P/C, Murphy et al. 1987)
29.60 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
8.24 (calculated-QSAR, Achman et al. 1993)
25.59 (calculated-QSPR, Dunnivant et al. 1992)
24.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
42.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.10 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.10 (recommended, Sangster 1993)
6.1262 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.15, 9.06	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.81	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.71	(suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.003 d^{-1} with $t_{1/2}$ = 219 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{1/2}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

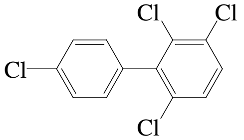
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 219 d for high-dose treatment, $t_{1/2}$ = 172 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.64 2,3,4′,6-Tetrachlorobiphenyl (PCB-64)



Common Name: 2,3,4′,6-Tetrachlorobiphenyl
Synonym: PCB-64, 2,3,4′,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4′,6-tetrachlorobiphenyl
CAS Registry No: 52663-58-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
57 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.130 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0937 (20°C, supercooled liquid, Murphy et al. 1987)
0.028 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0138 (P_L supercooled liquid, GC-RT correlation Burkhard et al. 1985a)
0.0146 (GC-RI correlation, Burkhard et al. 1985b)
5.51×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/mmHg) = 10.70 - 4510/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00776, 0.0141 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.30$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
31.01 (calculated-P/C, Burkhard 1984)
17.25 (20°C, calculated-P/C, Murphy et al. 1987)
28.37 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
14.2 (wetted-wall column-GC, Brunner et al. 1990)
27.59 (calculated-QSPR, Dunnivant et al. 1992)
24.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
42.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated-TSA, Burkhard 1984)
5.76 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0 (calculated-TSA, Murray & Andren 1992)
5.76 (recommended, Sangster 1993)
5.8251 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

8.41; 7.91 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)

log K_{OA} = –6.43 + 4420/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)

8.80 (quoted, Kömp & McLachlan 1997b)

9.62, 8.63; 8.74 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

8.54 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.64 (suspended particular matter, Burkhard 1984)

5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4 – 0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25 – 60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.005 d^{-1} with $t_{½}$ = 140 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 160 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

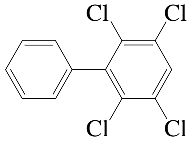
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 140 d for high-dose treatment, $t_{½}$ = 160 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.65 2,3,5,6-Tetrachlorobiphenyl (PCB-65)



Common Name: 2,3,5,6-Tetrachlorobiphenyl
Synonym: PCB-65, 2,3,5,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,5,6-tetrachlorobiphenyl
CAS Registry No: 33284-54-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
  77–77.5 (Bolgar 1973)
  79.0 (Burkhard 1984; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.295 (mp at 79°C)

Water Solubility (g/m^3 or mg/L at 25°C):
  0.162 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.0099, 0.0216, 0.0119, 0.0279 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
  0.0431 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.0151 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.00467 (GC-RI correlation, Burkhard et al. 1985b)
  0.0151 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
  $\log (P_L/Pa) = -4229/(T/K) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
  0.0238 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  27.26 (calculated-P/C, Burkhard 1984)
  31.01 (calculated-QSAR- MCI χ, Sabljic & Güsten 1989)
  34.10 (calculated-QSPR, Dunnivant et al. 1992)
  35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  5.77 (calculated-TSA, Burkhard 1984)
  6.07, 5.95, 5.98, 5.85 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  5.94; 5.86 (generator column-GC; calculated-TSA, Hawker & Connell 1988a)
  5.96 (recommended, Sangster 1993)
  7.8733 (calculated-UNIFAC group contribution method, Chen et al. 1993)

5.86 (recommended, Hansch et al. 1995)
5.81; 5.46–5.96 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
6.0133 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
5.83 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:
8.40 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

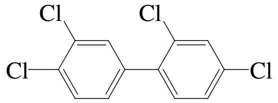
Bioconcentration Factor, log BCF or log K_B:
2.46 (*Poecillia reticulata*, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
5.57 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.4 – 0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:

7.1.1.66 2,3′,4,4′-Tetrachlorobiphenyl (PCB-66)



Common Name: 2,3′,4,4′-Tetrachlorobiphenyl
Synonym: PCB-66, 2,3′,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′-tetrachlorobiphenyl
CAS Registry No: 32598-10-0
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
  124 (Saeki et al. 1971; Hutzinger et al. 1974)
  127–127.5 (Webb & McCall 1972)
  127–128 (Wallnöfer et al. 1973, Bolgar 1973)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.105 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.058 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
  0.0168 (calculated-TSA, Mackay et al. 1980)
  0.098 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
  0.00474 (calculated-fragment solubility constants, Wakita et al. 1986)
  0.0368 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  0.068 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  0.0273 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
  0.0116 (calculated-TSA, Abramowitz & Yalkowsky 1990)
  0.045 (calculated-MCI χ, Patil 1991)
  0.00446 (calculated-QSPR, Dunnivant et al. 1992)
  0.0216 (calculated-group contribution method, Kühne et al. 1995)
  0.0266 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  0.00616 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
  0.000494 (GC-RI correlation, Burkhard et al. 1985a)
  0.00459 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  0.00569, 0.00507 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.00252 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  $\log (P/mmHg) = 10.90 - 4650/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
  0.00427, 0.0059 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
  $\log (P_L/Pa) = -4349/(T/K) + 12.38$ (GC-RT correlation, Falconer & Bidleman 1994)
  0.00347 (supercooled liquid P_L, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
  84.20 (calculated-P/C, Murphy et al. 1983)
  13.68 (calculated-P/C, Burkhard et al. 1985b)

14.18 (quoted, Eisenreich 1987)
20.37 (20°C, calculated-P/C, Murphy et al. 1987)
25.84 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
12.16 (wetted-wall column-GC, Brunner et al. 1990)
20.55 (calculated-QSPR, Dunnivant et al. 1992)
36.97* ± 0.48 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 7.4573 - 3488.7/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(29.0/kJ\cdot mol^{-1})/RT] + (0.062/kJ\cdot mol^{-1}\cdot K^{-1})/R]$; where $R = 8.314\ J\cdot K^{-1}\cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
35.4 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.90 (HPLC-RT correlation, Shaw & Connell 1982)
5.80, 6.31 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.98 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.31 (generator column-GC/ECD, Hawker & Connell 1988a)
6.09 (generator column-GC, Larsen et al.1992)
6.12 (recommended, Sangster 1993)
6.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
9.22* (20°C, generator column-GC, measured range 0–30°C, Harner & Bidleman 1996)
$\log K_{OA} = -3.82 + 3827/(T/K)$; temp range 0–30°C (generator column-GC, Harner & Bidleman 1996)
9.73 (10°C, estimated, Thomas et al. 1998)
10.33, 9.29; 9.22 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.36 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
4.45 (worms, Oliver 1987c)
3.18–4.62 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.55–5.76 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.80, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
5.74 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.72 (soil, calculated-S, Chou & Griffin 1986)
5.23 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.90 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
6.10 (organic carbon, obs., Murray & Andren 1992)
4.90 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
5.20 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Hydrolysis:
Photolysis: photodegradation $k = (0.11 \pm 0.02)\ h^{-1}$ with $t_{½} = 7.1$ h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.4 - 0.9) \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 5.1 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.001 d^{-1} (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

k_2 = 0.009 d^{-1} with $t_{1/2}$ = 82 d and k_2 = 0.013 d^{-1} with $t_{1/2}$ = 55 d for food concn of 21 ng/g and 158 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_2 = 0.004 d^{-1} with $t_{1/2}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.003 d^{-1} with $t_{1/2}$ = 225 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

photodegradation $t_{1/2}$ = (7.1 ± 1.5) h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.067 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.75 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.18 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.32 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00081 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.0024 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00443 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.000295 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{1/2}$ = 670 d in rainbow trout, and $t_{1/2}$ = 108 d its muscle (Niimi & Oliver 1983)

$t_{1/2}$ = 33 d in worms at 8°C(Oliver 1987c)

depuration $t_{1/2}$ = 55–82 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2}$ = 164 d for high-dose treatment, $t_{1/2}$ = 225 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.66.1
Reported Henry's law constants and octanol-air partition coefficients of 2,3′,4,4′-tetrachlorobiphenyl (PCB-66) at various temperatures and temperature dependence equations

Henry's law constant		**log K_{OA}**			
Bamford et al. 2000		**Harner & Bidleman 1996**		**Zhang et al. 1999**	
gas stripping-GC/MS		**generator column-GC**		**multicolumn-GC-k′ correlation**	
t/°C	**H/(Pa m³/mol)**	**t/°C**	**log K_{OA}**	**t/°C**	**log K_{OA}**
4	14.17	0	10.21	0	10.33
11	19.80	10	9.65	20	9.29
18	27.25	20	9.22		
25	36.97	30	8.82		
31	47.51				
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 73.28$			
$\ln K_{AW} = -\Delta H/RT + \Delta S/R$					
	K_{AW}	$\log K_{OA} = A + B/T$			
A	7.4573	A	−3.82		
B	3488.09	B	3827		
enthalpy, entropy change:					
$\Delta H/(\text{kJ·mol}^{-1}) = 29.0 \pm 2.6$					
$\Delta S/(\text{J·mol}^{-1}\text{·K}^{-1}) = 62 \pm 8$					

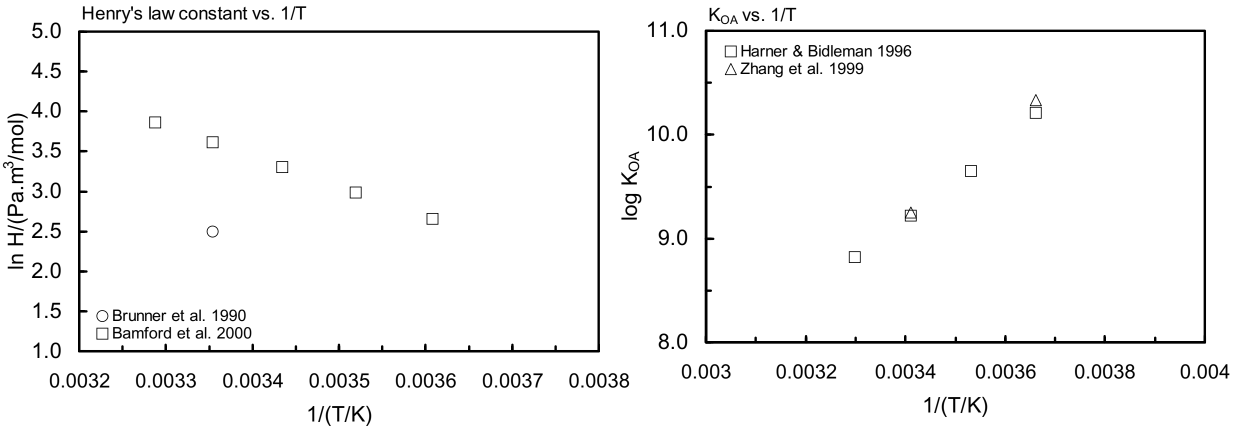
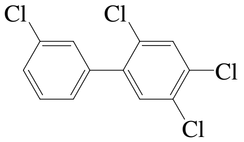


FIGURE 7.1.1.66.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,3′,4,4′-tetrachlorobiphenyl (PCB-66).

7.1.1.67 2,3′,4,5-Tetrachlorobiphenyl (PCB-67)



Common Name: 2,3′,4,5-Tetrachlorobiphenyl
Synonym: PCB-67, 2,3′,4,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,5-tetrachlorobiphenyl
CAS Registry No: 73575-53-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
83 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0987 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0351, 0.0298, 0.00804, 0.0266 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00654 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0070 (GC-RI correlation, Burkhard et al. 1985b)
$\log (P/mmHg) = 10.70 - 4530/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00708 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4382/(T/K) + 12.52$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
19.35 (calculated-P/C, Burkhard 1984)
29.18 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
23.70 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.93 (calculated-TSA, Burkhard 1984)
6.22, 6.32, 6.40, 6.33 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.32 (recommended, Sangster 1993)
6.2276 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.06 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.73 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

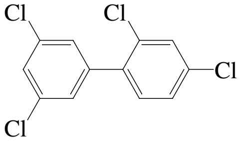
Ground water:

Sediment:

Soil:

Biota:

7.1.1.68 2,3′,4,5′-Tetrachlorobiphenyl (PCB-68)



Common Name: 2,3′,4,5′-Tetrachlorobiphenyl
Synonym: PCB-68
Chemical Name: 2,3′,4,5′-tetrachlorobiphenyl
CAS Registry No: 73575-52-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
71 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.085 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.00679 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00726 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
23.30 (calculated-P/C, Burkhard 1984)
55.02 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
38.17 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.99 (calculated-TSA, Burkhard 1984)
6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.2624 (calculated molecular properties MNDO-AM method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.66 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.79 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 11 (food lipid mg)/(g worm lipid-d); k_2 = 0.08 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

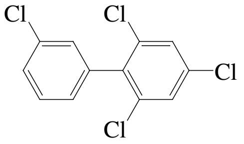
Ground water:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 8 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.69 2,3′,4,6-Tetrachlorobiphenyl (PCB-69)



Common Name: 2,3′,4,6-Tetrachlorobiphenyl
Synonym: PCB-69
Chemical Name: 2,3′,4,6-tetrachlorobiphenyl
CAS Registry No: 60233-24-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
45 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.105 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0097, 0.0146, 0.0184, 0.0243 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0169 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0179, (GC-RI correlation, Burkhard et al. 1985b)
$\log (P/mmHg) = 10.60 - 4440/T$ (GC-RT correlation, Tateya et al. 1988)
0.01911 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.43$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
47.12 (calculated-P/C, Burkhard 1984)
63.53 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
21.28 (wetted-wall column-GC/ECD, Brunner et al. 1990)
51.22 (calculated-QSAR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.09,6.06, 6.09, 5.89 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0068 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.47 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.71 (suspended particulate matter, Burkhard et al. 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

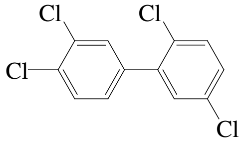
Ground water:

Sediment:

Soil:

Biota:

7.1.1.70 2,3′,4′,5-Tetrachlorobiphenyl (PCB-70)



Common Name: 2,3′,4′,5-Tetrachlorobiphenyl
Synonym: PCB-70, 2,3′,4′,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3′,4′,5-tetrachlorobiphenyl
CAS Registry No: 32598-11-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):

104	(Bellavita 1935; Hutzinger et al. 1974)
104–107	(Wallnöfer et al. 1973, Bolgar 1973)

Boiling Point (°C):

Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):

268.2	(calculated-Le Bas method at normal boiling point)
211.6	(Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.168 (mp at 104°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.041	(shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.029	(calculated-TSA, Mackay et al. 1980)
0.022	(generator column-GC, Bruggeman et al. 1981)
0.099	(supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0091	(generator column-GC/ECD, Opperhuizen et al. 1985)
0.0104	(calculated-fragment solubility constants, Wakita et al. 1986)
0.0362	(20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0254, 0.0368, 0.0432, 0.030	(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0273	(calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.0184	(calculated-TSA, Abramowitz & Yalkowsky 1990)
0.045	(calculated-MCI χ, Patil 1991)
0.0111	(calculated-QSPR, Dunnivant et al. 1992)
0.0114, 0.0306	(calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.0463	(calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00544, 0.00642	(supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
0.00769	(calculated S × HLC, Burkhard et al. 1985a)
0.000919	(GC-RI correlation, Burkhard et al. 1985a)
0.00519	(supercooled liquid P_L, calculated-GC-RI, Burkhard et al. 1985b)
0.00526, 0.00551	(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0060	(selected P_L, supercooled liquid, Shiu & Mackay 1986)

0.00236 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4640/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00447, 0.0063 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4431/(T/K) + 12.60 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
20.26 (calculated-P/C, Murphy et al. 1983)
15.30 (calculated-P/C, Burkhard et al. 1985b)
19.05 (20°C, calculated-P/C, Murphy et al. 1987)
19.15 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC, Brunner et al. 1990)
20.50 (calculated-QSPR, Dunnivant et al. 1992)
17.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = $-\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 29 ± 3 kJ/mol, ΔS_H = 0.06 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.95 (shake flask-GC, Tulp & Hutzinger 1978)
5.95 (HPLC-k′ correlation, McDuffie 1981)
6.39 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.30 (HPLC-RT correlation, Shaw & Connell 1982)
5.72, 6.23 (HPLC-RT correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.18 (HPLC-RT correlation, Opperhuizen et al. 1985)
6.01, 6.24, 6.36, 6.29 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.99 (generator column-GC, Larsen et al. 1992)
5.99 (HPLC-k′ correlation, Neogrohati & Hammers 1992)
5.7833 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.23 (recommended, Sangster 1993)
6.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.29, 9.22; 9.29 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.92 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:
6.15 (goldfish, 3% lipid, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
6.20 (goldfish, 3% lipid, calculated-K_{OW}, Bruggeman et al. 1981)
4.62, 5.11 (goldfish, exptl., correlated, Mackay & Hughes 1984)
4.32, 5.50 (guppy, lipid phase, Opperhuizen et al. 1985)
4.92 (guppy, Gobas et al. 1987)
4.62, 4.32 (fish, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
5.08; 6.61 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.32, 5.62; 4.742, 4.257 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
5.08, 6.61 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.70, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.02, 4.86, 4.85, 4.69 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
5.73 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.6–6.8, 6.3 (suspended sediment, average, Oliver 1987a)
7.20 (algae > 50 μm, Oliver 1987a)
4.81 (soil, calculated-S, Chou & Griffin 1986)
4.76 (correlated literature values in soils, Sklarew & Girvin 1987)
6.04 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.52 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.84 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
5.02; 5.07 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.30 (soil, calculated-K_{OW}, Girvin & Scott 1997)
4.86, 4.80 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\text{-}}$(aq.) = 5.5×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2}$ ~4–11 d in freshwater systems, 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 420 d^{-1}; k_2 = 0.01 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986, Clark et al. 1990))
k_2 = 0.01, 0.0104 d^{-1} (goldfish, exptl., correlated, Mackay & Hughes 1984)
k_1 = 380 d^{-1}; k_2 = 0.018 d^{-1} (guppy, Opperhuizen et al. 1985)
k_1 = 17.5 h^{-1}; $1/k_2$ = 2400 h (goldfish, quoted, Hawker & Connell 1985)
log k_1 = 2.58, 2.62 d^{-1}; log $1/k_2$ = 1.74, 2.0 d (fish, quoted, Connell & Hawker 1988)
log k_2 = –2.0 d^{-1} (fish, quoted, Thomann 1989)
k_1 = 3340 d^{-1}; k_2 = 0.0280 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_1 = 0.00043 h^{-1}; k_2 = 0.170 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1 = 10 (food lipid mg)/(g worm lipid-d); k_2 = 0.09 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{1/2}$ = 167 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{1/2}$ = 217 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
photodegradation $t_{½}$ = 4.87 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

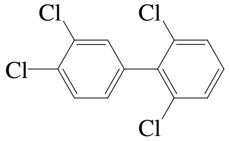
Groundwater:

Sediment:

Soil:

Biota: clearance $t_{½}$ = 60 d in goldfish (static equilibration system, 23-d exposure, Bruggeman et al. 1981)
$t_{½}$ = 38.6 d in guppy (Opperhuizen et al. 1985);
elimination $t_{½}$ = 8 d in earthworm given contaminated food (Wågman et al. 2001)
depuration $t_{½}$ = 167 d for high-dose treatment, $t_{½}$ = 217 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.71 2,3′,4′,6-Tetrachlorobiphenyl (PCB-71)



Common Name: 2,3′,4′,6-Tetrachlorobiphenyl
Synonym: PCB-71
Chemical Name: 2,3′,4′,6-tetrachlorobiphenyl
CAS Registry No: 41464-46-4
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
57 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.123 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0278 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.59×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)
0.0102 (GC-RI correlation, Burkhard et al. 1985b)
0.00912, 0.00877 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00776, 0.0115 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.14$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
22.80 (calculated-P/C, Burkhard 1984)
32.53 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
14.31 (calculated-QSPR, Achman et al. 1993)
31.82 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.86 (calculated-TSA, Burkhard 1984)
5.76 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.98 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.7206 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
9.78, 8.84; 8.98 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.66 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 5.7×10^9 dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

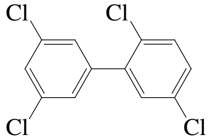
Ground water:

Sediment:

Soil:

Biota:

7.1.1.72 2,3′,5,5′-Tetrachlorobiphenyl (PCB-72)



Common Name: 2,3′,5,5′-Tetrachlorobiphenyl
Synonym: PCB-72
Chemical Name: 2,3′,5,5′-tetrachlorobiphenyl
CAS Registry No: 41464-42-0
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
56 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0861 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0107 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.66×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.00818, 0.00957 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.010, 0.00988 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P_L/Pa) = –4382/(T/K) + 12.70 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
25.34 (calculated-P/C, Burkhard 1984)
48.33 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
36.70 (calculated-QSAR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.98 (calculated, Burkhard 1984)
6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.2101 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.78 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4 – 0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

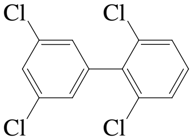
Ground water:

Sediment:

Soil:

Biota:

7.1.1.73 2,3′,5′,6-Tetrachlorobiphenyl (PCB-73)



Common Name: 2,3′,5′,6-Tetrachlorobiphenyl
Synonym: PCB-73
Chemical Name: 2,3′,5′,6-tetrachlorobiphenyl
CAS Registry No: 74338-23-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
66 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0142 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.0150, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
38.91 (calculated-P/C, Burkhard 1984)
61.81 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
52.69 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8026 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
7.97 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–0 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–0 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

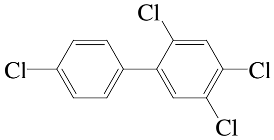
Ground water:

Sediment:

Soil:

Biota:

7.1.1.74 2,4,4′,5-Tetrachlorobiphenyl (PCB-74)



Common Name: 2,4,4′,5-Tetrachlorobiphenyl
Synonym: PCB-74, 2,4,4′,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,4,4′,5-tetrachlorobiphenyl
CAS Registry No: 32690-93-0
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
125 (Burkhard et al. 1985a; Shiu & Mackay 1986; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.102 (calcd-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0978 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0306 (20°C, supercooled liquid, Murphy et al. 1987)
0.0496 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0116 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00453 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0058 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00209, 0.000636, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00731, 0.00692 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.12×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 10.80 - 4600/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00479, 0.00631 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4382/(T/K) + 12.56$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0116 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
17.33 (calculated-P/C, Burkhard 1984)
21.18 (20°C,calculated-P/C, Murphy et al. 1987)
21.18 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
21.76 (calculated-QSPR, Dunnivant et al. 1992)
23.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.16, 6.67	(HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.10	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.10	(recommended, Sangster 1993)
6.67	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.25, 9.14; 8.96	(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.38–9.65	(10°C, estimated, Thomas et al. 1998)
9.11	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:

51	(trout in Lake Ontario, Niimi 1996)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 4.90	(Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.60	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:

5.74	(suspended particulate matter, Burkhard 1984)
6.30	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.0	(soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.50	(soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 5.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{½}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.003 d^{-1} with $t_{½}$ = 220 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

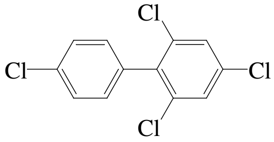
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 172 d for high-dose treatment, $t_{½}$ = 220 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.75 2,4,4′,6-Tetrachlorobiphenyl (PCB-75)



Common Name: 2,4,4′,6-Tetrachlorobiphenyl
Synonym: PCB-75, 2,4,4′,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,4,4′,6-tetrachlorobiphenyl
CAS Registry No: 32598-12-2
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
93.0 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.104 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.00967, 0.0127, 0.0122, 0.0180 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.091 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.045 (calculated-MCI χ, Patil 1991)
0.0804 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0204, 0.0158, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0150 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0179, 0.0202 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/\text{Pa}) = -4229/(T/\text{K}) + 12.44$ (GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
42.25 (calculated-P/C, Burkhard et al. 1985b)
42.25 (batch stripping, Dunnivant & Elzerman 1988)
55.32 (calculated- QSPR-MCI χ, Sabljic & Güsten 1989)
47.07 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.08, 6.10, 5.97, 5.97 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.03 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

8.19	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.72	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

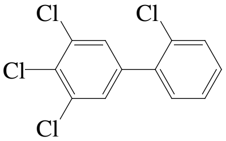
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.76 2,3′,4′,5′-Tetrachlorobiphenyl (PCB-76)



Common Name: 2,3′,4′,5′-Tetrachlorobiphenyl
Synonym: PCB-76, 2,3′,4′,5′-tetrachlorobiphenyl
Chemical Name: 2,3′,4′,5′-tetrachlorobiphenyl
CAS Registry No: 70362-48-0
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
89 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.114 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0551 (20°C, supercooled liquid, Murphy et al. 1987)
0.0569 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0150 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.00512, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00602, 0.00426 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.44×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.00447, 0.00646 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4382/(T/K) + 12.48$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
12.16 (calculated-P/C, Burkhard 1984)
12.97 (20°C, calculated-P/C, Murphy et al. 1987)
22.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
10.13 (calculated-QSPR, Achman et al. 1993)
24.19 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.88 (calculated-TSA, Burkhard 1984)
5.98 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.05 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.23 (Hawker & Connell 1988b)
5.90 (calculated-QSPR, Murray & Andren 1992)

5.98	(recommended, Sangster 1993)
6.0763	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

8.93	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.68	(suspended particulate matter, Burkhard 1984)
6.0	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}$(aq.) = 5.5×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.005 d^{-1} with $t_{½}$ = 153 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

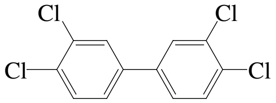
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 153 d for high-dose treatment, $t_{½}$ = 164 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.77 3,3′,4,4′-Tetrachlorobiphenyl (PCB-77)



Common Name: 3,3′,4,4′-Tetrachlorobiphenyl
Synonym: PCB-77, 3,3′,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 3,3′,4,4′-tetrachlorobiphenyl
CAS Registry No: 32598-13-3
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
 180 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
 268.2 (calculated-Le Bas method at normal boiling point)
 211.6 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 27.10 (Ruelle et al. 1993)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 56.6 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
 0.029 (calculated, assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)
 0.0202 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 0.175 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
 7.50×10^{-4} (generator column-GC/ECD, Weil et al. 1974)
 5.69×10^{-4}* (generator column-GC/ECD, measured 4–32°C, Dickhut et al. 1986)
 5.84×10^{-4}* (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
 $\ln x = -6098/(T/K) - 3.586$, temp range 4–32°C, ΔH_{ss} = 50.7 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
 $\log x = -2636/(T/K) - 1.558$, ΔH_{ss} = 50.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
 $S/(mol/L) = 3.59 \times 10^{-10} \exp(0.072 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
 8.23×10^{-4}, 1.01×10^{-3}, 1.16×10^{-3} (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 0.0018 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
 5.50×10^{-4}; 0.0161 (generator column-GC; supercooled liquid S_L, Dunnivant & Elzerman 1988)
 6.10×10^{-4} (generator column-GC/ECD, room temp., Hong & Qiao 1995)
 2.02×10^{-3}, 5.44×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
 $\log S_L$ (mol/L) = – 0.246 + 1339/(T/K) (supercooled liquid, Passivirta et al. 1999)
 $\ln x = -3.58245 - 6074.34/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
 0.00270* (generator column-GC/ECD, measured range 5–35°C. Huang & Hong 2002).—See Comment by van Noort 2004

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
 0.00219, 0.00196 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
 0.0014 (supercooled liquid P_L, GT-RT correlation, Burkhard 1984)

5.97×10^{-4}; 4.46×10^{-5}, 8.04×10^{-4} (calculated-MW, GC-RT correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0014 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00213, 0.00144 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.88×10^{-5}; 0.0020 (selected P_S, supercooled liquid P_L, Shiu & Mackay 1986)
0.00212 (supercooled liquid P_L, Dunnivant & Elzerman 1988)
1.82×10^{-5}; 5.26×10^{-4} (calculated-S × HLC, solid P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
0.00141, 0.00191(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4552/(T/K) + 12.61$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
1.202×10^{-3} (supercooled liquid P_L, 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
6.46×10^{-5}; 2.21×10^{-3} (solid, supercooled liquid, Passivirta et al. 1999)
$\log (P_S/Pa) = 15.56 - 5889/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 12.61 - 4552/(T/K)$ (liquid, Passivirta et al. 1999)
$(1.82 - 80.4) \times 10^{-5}$; $(4.71 - 22.0) \times 10^{-4}$ (quoted lit. P_S range; lit. P_L range, Delle Site 1997)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4.37 (calculated-P/C, Burkhard et al. 1985b)
1.72 (calculated-P/C, Shiu & Mackay 1986)
9.52 (gas stripping-GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
40.88 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.39 (calculated-QSPR, Dunnivant et al. 1992)
$\log H (Pa\ m^3/mol) = 12.86 - 3214/(T/K)$ (Passivirta et al. 1999)
16.20* ± 0.41 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 11.0657 - 4787.1/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(39.8/kJ \cdot mol^{-1})/ RT] + (0.092/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where $R = 8.314\ J \cdot K^{-1} \cdot mol^{-1}$ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
16.7 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 40 \pm 6$ kJ/mol, $\Delta S_H = 0.09 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.04 (HPLC-RT correlation, Sugiura et al. 1979)
6.52 (RP-TLC-retention, Bruggeman et al. 1982)
5.62 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.77 (HPLC-k′ correlation, De Kock & Lord 1987)
6.11, 6.40, 6.37 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.21 (generator column-GC, Hawker & Connell 1988a)
6.630 ± 0.018 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
6.13 (generator column-GC, Larsen et al. 1992)
5.98 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.11 (recommended, Sangster 1993)
6.63 (recommended, Hansch et al. 1995)
6.48 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

9.08 (calculated, Paterson et al. 1991)
9.96* (20°C, generator column-GC, measured range 0 to 30°C, Harner & Bidleman 1996)
$\log K_{OA} = -3.14 + 3828/(T/K)$; (temp range 0 to 30°C, Harner & Bidleman 1996)
10.92, 9.92; 10.03 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

9.70 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.29; 9.19 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.46 (killifish, Goto et al. 1978)
3.90, 3.24, 3.63, 4.15 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
2.77, 2.63 (human fat in lipid, wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
5.36; 6.89 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.59, 5.87; 4.745, 4.943 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
2.56–4.26 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.19–5.23 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.36 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
5.36, 6.90 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.41, 6.37 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
2.62, 2.77 (human: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.75 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.41 (soil, calculated, Chou & Griffin 1986)
5.02 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.029, 0.0047 d^{-1} (golden orfe, guppy, Sugiura et al. 1979)
k_2 = 0.0157 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 5160 d^{-1}; k_2 = 0.0224 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_1 = 17 L d^{-1} g^{-1} dry wt.; k_2 = 0.073 d^{-1} (Baltic Sea blue mussel, flow-through expt., Gustafsson et al. 1999)
k_2 = 0.0251 d^{-1} with $t_{½}$ = 28 d (newly contaminated oysters, Gardinali et al. 2004)
k_2 = 0.0166 d^{-1} with $t_{½}$ = 42 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995);
$t_{½}$ = 1500 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: $t_{½}$ = 805 d in Lake Michigan (Neely 1983);
photodegradation $t_{½}$ = 528 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996);
$t_{½}$ = 30000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{1/2}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{1/2}$ = 44 d in rainbow trout, and its muscle, 29 d (Niimi & Oliver 1983);

theoretical half-life to reach 90% steady-state tissue concn 9.5 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)

Depuration $t_{1/2}$ = 28 d for newly contaminated oysters, and $t_{1/2}$ = 42 d for chronically contaminated oysters (Gardinali et al. 2004)

TABLE 7.1.1.77.1

Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 3,3′,4,4′-tetrachlorobiphenyl (PCB 77) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility				Henry's law constant		log K_{OA}	
Dickhut et al. 1986		Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$H/(Pa\ m^3/mol)$	t/°C	log K_{OA}
4	1.46×10^{-4}	5	1.25×10^{-3}	4	4.46	0	10.88
20	4.38×10^{-4}	15	1.77×10^{-3}	11	6.99	10	10.36
25	5.84×10^{-4}	25	2.70×10^{-3}	18	10.75	20	9.96
32	1.17×10^{-3}	35	4.35×10^{-3}	25	16.20	30	9.47
				31	22.69		
ln x = A − B/(T/K)		mp/°C	180–181			$\Delta H_{OA}/(kJ\ mol^{-1})$ = 73.30	
A	−3.586			enthalpy, entropy change:			
B	6098.15	$\Delta H_{sol}/(kJ\ mol^{-1})$ = 29.6		$\Delta H/(kJ\cdot mol^{-1})$ = 39.8 ± 6.0		log K_{OA} = A + B/T	
				$\Delta S/(J\cdot mol^{-1}\cdot K^{-1})$ = 92 ± 20		A	−3.14
enthalpy of solution:						B	3828
$\Delta H_{sol}/(kJ\ mol^{-1})$ = 50.7 ± 4.8				ln K_{AW} = −ΔH/RT + ΔS/R			
	for 4–32°C			A	11.6567		
				B	4787.11		

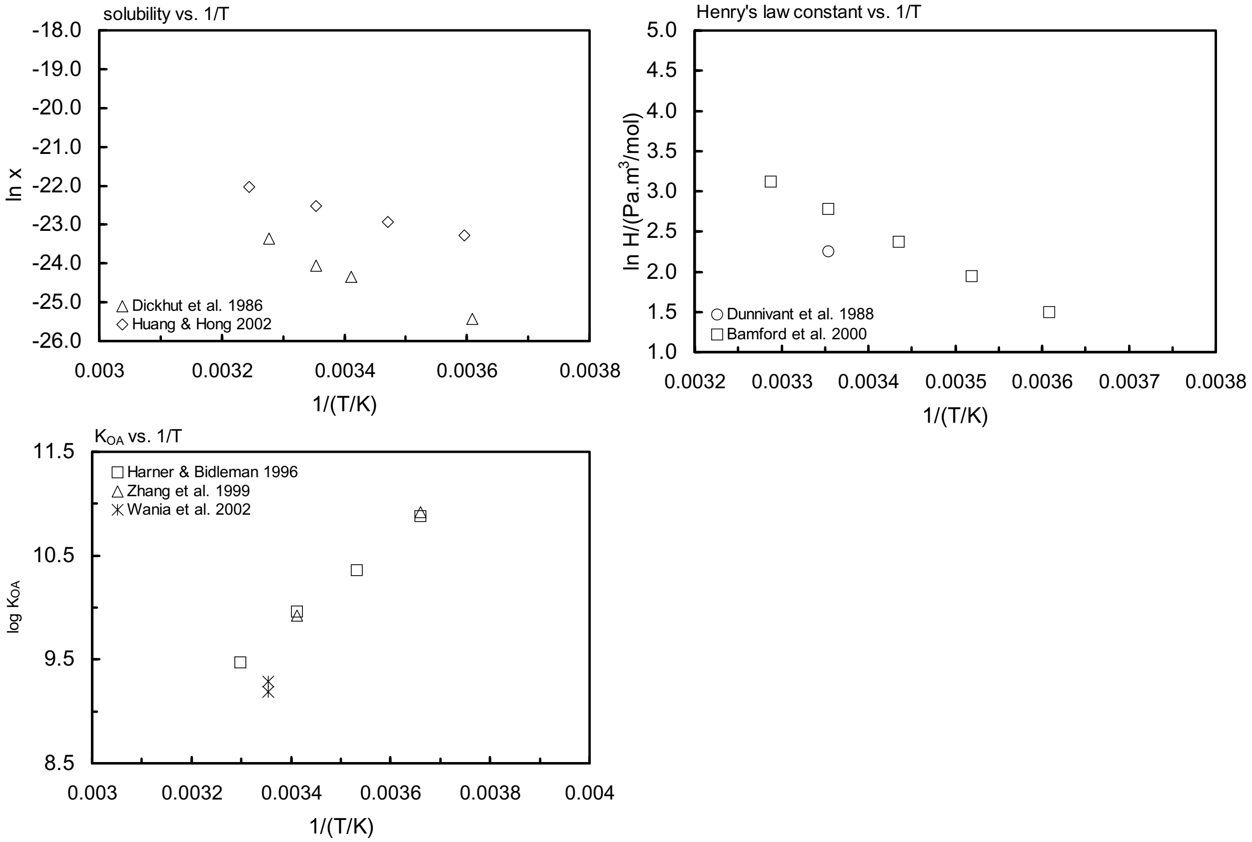
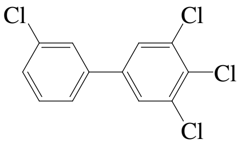


FIGURE 7.1.1.77.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 3,3′,4,4′-tetrachlorobiphenyl (PCB-77).

7.1.1.78 3,3′,4,5-Tetrachlorobiphenyl (PCB-78)



Common Name: 3,3′,4,5-Tetrachlorobiphenyl
Synonym: PCB-78
Chemical Name: 3,3′,4,5-tetrachlorobiphenyl
CAS Registry No: 70362-49-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
  94 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
  0.0943 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.00923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.00186 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.00116, 0.000167, 0.000223 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
  0.00319, 0.00206 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  $\log (P_L/\text{Pa}) = -4598/T + 12.92$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
  5.76 (calculated-P/C, Burkhard 1984)
  22.90 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  21.77 (calculated-QSPR, Dunnivant et al. 1992)
  20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  5.95 (calculated, Burkhard 1984)
  6.35 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
  6.2278 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
  5.75 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1: 8 (food lipid mg)/(g worm lipid-d); k_2: 0.09 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

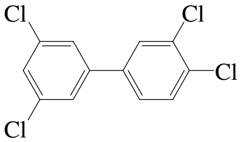
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2}$ = 7 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.79 3,3′,4,5′-Tetrachlorobiphenyl (PCB-79)



Common Name: 3,3′,4,5′-Tetrachlorobiphenyl
Synonym: PCB-79
Chemical Name: 3,3′,4,5′-tetrachlorobiphenyl
CAS Registry No: 41464-48-6
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):

83	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

268.2	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0815	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00923	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0036	(calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

2.07×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.00224, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00341, 0.00206 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4598/(T/K) + 12.95$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

7.39	(calculated-P/C, Burkhard 1984)
11.75	(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
3.94	(calculated-QSPR, Achman et al. 1993)
12.73	(calculated-QSAR, Dunnivant et al. 1992)
20.8	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.00	(calculated-TSA, Burkhard 1984)
6.42	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.3035	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.67	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.80 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

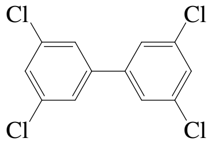
Ground water:

Sediment:

Soil:

Biota:

7.1.1.80 3,3′,5,5′-Tetrachlorobiphenyl (PCB-80)



Common Name: 3,3′,5,5′-Tetrachlorobiphenyl
Synonym: PCB-80, 3,3′,5,5′-tetrachloro-1,1′-biphenyl
Chemical Name: 3,3′,5,5′-tetrachlorobiphenyl
CAS Registry No: 33284-52-5
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
164 (Van Roosmalen 1934; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0421 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0712 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.000306, 0.000496, 0.000786, 0.000902 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00124 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0295 (supercooled liquid S_L, calculated-mp, Dunnivant & Elzerman 1988)
0.00292 (calculated-TSA, Abramowitz & Yalkowsky 1990)
2.92×10^{-3}, 7.68×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
4.96×10^{-3} (calculated–mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.000859, 0.000139, 0.0219 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00305 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00547, 0.00511 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/\text{Pa}) = -4598/(T/K) + 13.16$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
12.46 (calculated-P/C, Burkhard et al. 1985b)
63.02 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
38.0 (calculated-QSPR, Dunnivant et al. 1992)
20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.85 (HPLC-RT correlation, Sugiura et al. 1978; quoted, Hansch et al. 1995)
6.58 (RP-TLC-retention, Bruggeman et al. 1982)

6.77, 6.77, 6.45, 6.41 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.60 (recommended, Sangster 1993)
6.48, 6.85 (quoted lit. values, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.26 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

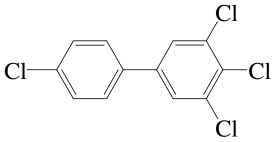
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
5.85 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

7.1.1.81 3,4,4′,5-Tetrachlorobiphenyl (PCB-81)



Common Name: 3,4,4′,5-Tetrachlorobiphenyl
Synonym: PCB-81
Chemical Name: 3,4,4′,5-Tetrachlorobiphenyl
CAS Registry No: 70362-50-4
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
  137 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  0.0929 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985)
  0.00292 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
  0.0010 (room temp., generator column-GC/ECD, Hong & Qiao 1995)—see comment by van Noort 2004
  0.00313 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)
  0.00140, 0.00213, 0.00313, 0.00505 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.00165 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.0204, 0.0018, 0.00804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
  0.00290, 0.00182. (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  $\log (P_L/Pa) = -4598/(T/K) + 12.88$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  5.20 (calculated-P/C, Burkhard et al. 1985a)
  15.0 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  10.06 (calculated-QSPR, Dunnivant et al. 1992)
  5.97 (calculated-QSPR, Achman et al. 1993)
  12.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  25.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 33 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  5.96 (calculated-TSA, Burkhard 1984)
  6.36 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
  6.1949 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
  6.53; 6.16 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
  6.64, 6.24 (calculated-MCI χ, calculated-molecular properties MNDO-MI method, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.88 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.10, 6.40 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.0185$ d^{-1} with $t_{½}$ = 37 d (newly contaminated oysters, Gardinali et al. 2004)

$k_2 = 0.0186$ d^{-1} with $t_{½}$ = 37 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

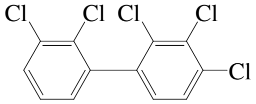
Soil:

Biota: clearance $t_{½}$ = 21 d in guppy for tetrachlorobiphenyl (Bruggeman et al. 1984);

reported biological half-lives for tetrachlorobiphenyls: $t_{½}$ = 2–290 d in trout, $t_{½}$ = 29–127 d in trout muscle; $t_{½}$ = 51–81 d in goldfish, $t_{½}$ = 7–200 d in carp and $t_{½}$ = 4–53 d in guppy (Niimi 1987)

Depuration $t_{½}$ = 37 d for newly contaminated oysters, and $t_{½}$ = 37 d for chronically contaminated oysters (Gardinali et al. 2004)

7.1.1.82 2,2′,3,3′,4-Pentachlorobiphenyl (PCB-82)



Common Name: 2,2′,3,3′,4-Pentachlorobiphenyl
Synonym: PCB-82
Chemical Name: 2,2′,3,3′,4-pentachlorobiphenyl
CAS Registry No: 52663-62-4
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
85 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0467 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0291 (20°C, supercooled liquid, Murphy et al. 1987)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0028 (calculated-QSPR, Dunnivant et al. 1992)
0.00622 (calculated-group contribution method, Kühne et al. 1995)
0.0221 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0020 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00218, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.06×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.0 – 4780/(T/K) (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
12.46 (calculated-P/C, Burkhard 1984)
11.86 (20°C, calculated-P/C, Murphy et al. 1987)
12.36 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
14.82 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
16.3 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 8$ kJ/mol, $\Delta S_H = 0.11 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.20 (calculated-TSA, Burkhard 1984)
6.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.30 (estimated, Girvin & Scott 1997)
6.0458 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.73 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.16 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.00 (suspended particulate matter, Burkhard 1984)

4.770 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

5.80 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{½}$ = 174 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 196d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

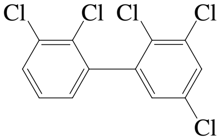
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 174 d for high-dose treatment, $t_{½}$ = 196 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.83 2,2′,3,3′,5-Pentachlorobiphenyl (PCB-83)



Common Name: 2,2′,3,3′,5-Pentachlorobiphenyl
Synonym: PCB-83
Chemical Name: 2,2′,3,3′,5-pentachlorobiphenyl
CAS Registry No: 60145-20-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):

65	(Ruelle & Kesselring 1997)

Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):

289.1	(calculated-Le Bas method at normal boiling point)
224.5	(Ruelle et al. 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.405 (mp at 65°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.0045	(generator column-GC/ECD, Weil et al. 1974)
0.023	(shake flask-GC/ECD, Wallnöfer et al. 1973)
0.046	(supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0282	(20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0260	(calculated-TSA, Abramowitz & Yalkowsky 1990)
0.0103, 0.0278	(calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.00735, 0.00324, 0.00278	(calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00299	(supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00274, 0.00303	(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00154	(20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log(P/\text{mmHg}) = 11.0 - 4760/(T/K)$	(GC-RT correlation, Tateya et al. 1988)
0.00204	(supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log(P_L/\text{Pa}) = -4522/(T/K) + 12.60$	(supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

21.28	(calculated-P/C, Burkhard et al. 1985b)
16.62	(20°C, calculated-P/C, Murphy et al. 1987)
26.65	(calculated- QSPR-MCI χ, Sabljic & Güsten 1989)
21.46	(calculated-QSPR, Dunnivant et al. 1992)
23.6	(11°C, gas stripping-GC/ECD, Bamford et al. 2002)
45.4	(from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 6$ kJ/mol, $\Delta S_H = 0.07 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.24	(calculated-TSA, Burkhard 1984)
6.26	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.51	(calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
6.0458	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.44, 9.39	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.01	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.04	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.748	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.004$ d^{-1} with $t_{1/2} = 172$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d^{-1} with $t_{1/2} = 217$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1996).

Surface water:

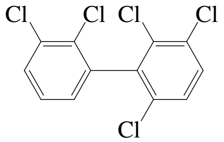
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 172$ d for high-dose treatment, $t_{1/2} = 217$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.84 2,2′,3,3′,6-Pentachlorobiphenyl (PCB-84)



Common Name: 2,2′,3,3′,6-Pentachlorobiphenyl
Synonym: PCB-84, 2,2′,3,3′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,6-pentachlorobiphenyl
CAS Registry No: 52663-60-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
91 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.047 (20°C, supercooled liquid, Murphy et al. 1987)
0.0542 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.48×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00693, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00372, 0.00441 supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.64×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 11.0 - 4740/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00302, 0.0055 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4399/(T/K) + 12.32$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
51.68 (calculated-P/C, Burkhard 1984)
17.63 (20°C,calculated-P/C, Murphy et al. 1987)
24.82 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
5.97 (calculated-QSPR, Achman et al. 1993)
25.45 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.04 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
5.60 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.24 (generator column-GC, Larsen et al. 1992)
5.96 (recommended, Sangster 1993)
6.04 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log $K_{OA} = -5.84 + 4360/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.80 (quoted, Kömp & McLachlan 1997b)
10.28, 9.28 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.94 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

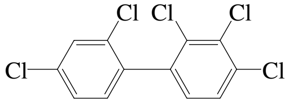
Biota Sediment Accumulation Factor, BSAF:
80 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:
6.09 (suspended particulate matter, Bukhard 1984)
4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH\text{-}}$(aq.) = 4.7 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.005 d^{-1} with $t_{½}$ = 135 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.005 d^{-1} with $t_{½}$ = 141 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 135 d for high-dose treatment, $t_{½}$ = 141 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.85 2,2′,3,4,4′-Pentachlorobiphenyl (PCB-85)



Common Name: 2,2′,3,4,4′-Pentachlorobiphenyl
Synonym: PCB-85, 2,2′,3,4,4′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′-pentachlorobiphenyl
CAS Registry No: 65510-45-4
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
87 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0428 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0219 (20°C, supercooled liquid, Murphy et al. 1987)
0.00782 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00233 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00253, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00472, 0.00218 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.12×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P_L/Pa) = -4522/(T/K) + 12.54$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.00248 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
17.83 (calculated-P/C, Burkhard 1984)
16.72 (20°C, calculated-P/C, Murphy et al. 1987)
24.82 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
6.69 (wetted-wall column-GC/ECD, Brunner et al. 1990)
19.49 (calculated-QSPR, Dunnivant et al. 1992)
26.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
47.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 7$ kJ/mol, $\Delta S_H = 0.05 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.61 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
6.18 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.18 (recommended, Sangster 1993)
6.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

9.29	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.07	(suspended particulate matter, Burkhard 1984)
4.748	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)
5.90	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.70	(soil-organic carbon, Girvin & Scott 1997)
5.51	(soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.70	(soil, calculated-$K_{OW,}$ Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

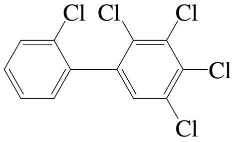
Ground water:

Sediment:

Soil:

Biota:

7.1.1.86 2,2′,3,4,5-Pentachlorobiphenyl (PCB-86)



Common Name: 2,2′,3,4,5-Pentachlorobiphenyl
Synonym: PCB-86, 2,2′,3,4,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5-pentachlorobiphenyl
CAS Registry No: 55312-69-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
100 (Mackay et al. 1980; Burkhard et al. 1985a; Opperhuizen et al. 1988; Brodsky & Ballschmiter 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.181 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0098 (generator column-GC/ECD, Weil et al. 1974)
0.0349 (generator column-HPLC/UV, Huang 1983)
0.034 (generator column-HPLC, Billington et al. 1988)
0.00334, 0.00554, 0.00297, 0.00651 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00933 (quoted, Neely 1981)
0.051 (P_L calculated from P_S using fugacity ratio F, Neely 1981)
0.00643 (supercooled liquid P_L, Neely 1981)
0.000077 (calculated, Neely 1983; quoted, Erickson 1986)
0.00133, 0.00245, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0128 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00288 (supercooled liquid P_L, GC-RI correlations, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4522/(T/\text{K}) + 12.61$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
84.1 (calculated-P/C, Burkhard et al. 1985b)
17.23 (calculated-MCI χ, Sabljic & Güsten 1989)
24.14 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.38 (Neely 1983; quoted, Erickson 1986)
7.49 (calculated-fragment const., Yalkowsky et al. 1983)
6.22 (calculated-TSA, Burkhard 1984)

6.38 (calculated-π const., Woodburn et al. 1984)
6.20 (selected, Shiu & Mackay 1986)
6.44, 6.38, 6.43, 6.29 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.23 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.26 (calculated-MCI χ, Patil 1991)
6.39 (recommended, Sangster 1993)
6.325 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.97 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/air Partition Coefficient, log K_{OA}:
9.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

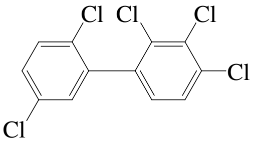
Bioconcentration Factor, log BCF:
4.43 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)

Sorption Partition Coefficient, log K_{OC}:
6.02 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.770 (marine humic substances, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.2 - 0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.3 - 0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Biodegradation: microbial degradation with pseudo first-order rate constant k = 0.005 yr^{-1} in the water column and k = 0.05 yr^{-1} in the sediment (Furukawa et al. 1978; quoted, Neely 1981).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water: $t_{½}$ = 108 d in Lake Michigan (Neely 1983).
Groundwater:
Sediment:
Soil:
Biota:

7.1.1.87 2,2′,3,4,5′-Pentachlorobiphenyl (PCB-87)



Common Name: 2,2′,3,4,5′-Pentachlorobiphenyl
Synonym: PCB-87, 2,2′,3,4,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5′-pentachlorobiphenyl
CAS Registry No: 38380-02-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
111.5–113 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2803
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.132 (Mackay et al. 1980)
0.138 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.022 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.0045 (generator column-GC/ECD, Weil et al. 1974)
0.0294 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0082, 0.00783, 0.00543, 0.0070 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00226 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.000392 (GC-RI correlation, Burkhard et al. 1985a)
0.00141, 0.00262 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00261, 0.00248 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00116 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.10 – 4800/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0017, 0.00275(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4562/(T/K) + 12.66 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
33.44 (calculated, Murphy et al. 1983)
19.86 (calculated-P/C, Burkhard et al. 1985b)
24.81 (calculated-P/C, Shiu & Mackay 1986)
12.87 (20°C, calculated-P/C, Murphy et al. 1987)
18.24 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
7.50 (wetted-wall column-GC, Brunner et al. 1990)
18.61 (calculated-QSPR, Dunnivant et al. 1992)
5.966 (calculated-QSPR, Achman et al. 1993)

37.71 ± 0.69 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
12.97, 18.83, 26.86, 37.71, 49.80 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 8.9006 – 3909.07/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(32.5/\text{kJ·mol}^{-1})/RT] + (0.074/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 $\text{J·K}^{-1}\text{·mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
36.5 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 33 ± 4 kJ/mol, ΔS_H = 0.07 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.85 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.30 (HPLC-RT correlation, Shaw & Connell 1982)
5.45, 6.37 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
6,63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.14, 6.23, 6.24, 6.27 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.36 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.23 (recommended, Sangster 1993)
6.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
9.96 (10°C, estimated, Thomas et al. 1998)
9.25 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:
4.43 (oyster, Vreeland 1974)
5.38; 6.91 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:
4.54 (Koch 1983)
6.07 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.88 (calculated, Bahnick & Doucette 1988)
4.761, 4.748 (marine humic substances of 5 mg/L DOC, selected, calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
4.76, 4.87, 4.85, 3.75 (marine humic substance in concentrations. of 5,10, 20, 40 mg/L DOC, reported as log K_h, Lara & Ernst 1989)
6.18 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.08 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.73 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted and selected, Baker et al. 2000)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.62 (soil, calculated-MCI, Sabljic et al. 1995)
5.02 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
6.00 (soil, calculated-K_{OW}, Girvin & Scott 1997)
5.80; 4.50 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Sorption Partition Coefficient, log K_{OM}:
4.50, 4.85 (selected, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2 – 0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3 – 0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.0045 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

k_1 = 0.049 h^{-1}; k_2 = 0.013 h^{-1} (mayfly-sediment model II, Gobas et al. 1989)

k_1 = 3360 d^{-1}; k_2 = 0.0140 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.005 d^{-1} with $t_{½}$ = 154 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 195 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

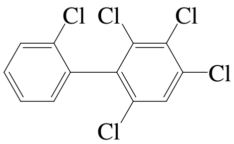
Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.027 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.57 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, and k = 0.27 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00152 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00223 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, and k = 0.0039 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{½}$ = 155 d in rainbow trout and $t_{½}$ = 62 d its muscle (Niimi & Oliver 1983).

depuration $t_{½}$ = 154 d for high-dose treatment, $t_{½}$ = 195 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.88 2,2′,3,4,6-Pentachlorobiphenyl (PCB-88)



Common Name: 2,2′,3,4,6-Pentachlorobiphenyl
Synonym: PCB-88
Chemical Name: 2,2′,3,4,6-pentachlorobiphenyl
CAS Registry No: 55215-17-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
100 (Mackay et al. 1980; Burkhard et al. 1985a; Opperhuizen et al. 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2803
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.182 (Mackay et al. 1980)

Water Solubility (g/m^3 or mg/L at 25°C):
0.012 (generator column-GC/ECD, Weil et al. 1974)
0.0129 (calculated-TSA, Mackay et al. 1980)
0.0385 (supercooled liquid S_L, calculated- TSA, Burkhard et al. 1985b)
0.00242 (calculated-fragment solubility constants, Wakita et al. 1986)
0.009 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.0206 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011 (calculated-MCI χ, Patil 1991)
0.00801 (calculated-group contribution, Kühne et al. 1995)
0.0124, 0.00472 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.0265 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00309 (GC-RI correlation, Burkhard et al. 1985a)
0.0161 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00646 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4399/(T/K) + 12.53$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
136.8 (calculated-P/C, Burkhard et al. 1985b)
34.65 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
38.97 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)–see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.51 (calculated-fragment const., Yalkowsky et al. 1983)

6.31	(calculated-TSA, Burkhard 1984)
6.07	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.26	(calculated-MCI χ, Patil 1991)
6.1452	(calculated-molecular properties, MNDO-AM1 method, Makino 1998)
6.84	(calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.39	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.11	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.611	(marine humic substances, calculated-MCI χ, reported as association coefficient log K_h at 5 mg/L of DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

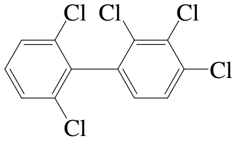
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.89 2,2′,3,4,6′-Pentachlorobiphenyl (PCB-89)



Common Name: 2,2′,3,4,6′-Pentachlorobiphenyl
Synonym: PCB-89, 2,2′,3,4,6′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,6′-pentachlorobiphenyl
CAS Registry No: 73575-57-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0382 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0542 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0206 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
4.82×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00522 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
41.64 (calculated-P/C, Burkhard 1984)
29.49 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
30.18 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
30.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 21 \pm 6$ kJ/mol, $\Delta S_H = 0.04 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.31 (calculated-TSA, Burkhard 1984)
6.07 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.60 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.40 (calculated-TSA, Murray & Andren 1992)
5.60 (recommended, Sangster 1993)
5.8981 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.11	(suspended particulate matter, Burkhard 1984)
4.611	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)
5.90	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

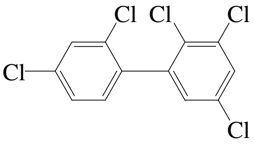
Ground water:

Sediment:

Soil:

Biota:

7.1.1.90 2,2′,3,4′,5-Pentachlorobiphenyl (PCB-90)



Common Name: 2,2′,3,4′,5-Pentachlorobiphenyl
Synonym: PCB-90, 2,2′,3,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5-pentachlorobiphenyl
CAS Registry No: 68194-07-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
67 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0375 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01344 (20°C, supercooled liquid S_L, Murphy et al. 1987)
0.00494 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00714 (calculated-group contribution method, Kühne et al. 1995)
0.00107, 0.00198 (generator column-GC/ECD, estimated, Hong & Qiao 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00375 (GC-RI correlation, Burkhard et al. 1985b)
$\log (P/\text{mmHg}) = 11.0 - 4740/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00347 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4522/(T/K) + 12.69$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
30.19 (calculated-P/C, Burkhard 1984)
39.11 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
29.83 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.32 (calculated-TSA, Burkhard 1984)
6.32 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988a)
6.36 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.32 (recommended, Sangster 1993)
6.339 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.92 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.12 (suspended particulate matter, Burkhard 1984)

4.66, 4.68, 4.75, 3.75 (marine humic substance in concentrations of 5,10, 20, 40 mg/L DOC, reported as log K_h, Lara & Ernst 1989)

4.659, 4.726 (marine humic substance, observed, calculated-MCI, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

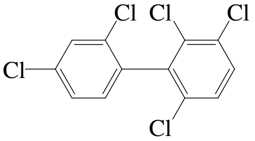
Ground water:

Sediment:

Soil:

Biota:

7.1.1.91 2,2′,3,4′,6-Pentachlorobiphenyl (PCB-91)



Common Name: 2,2′,3,4′,6-Pentachlorobiphenyl
Synonym: PCB-91, 2,2′,3,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,6-pentachlorobiphenyl
CAS Registry No: 58194-05-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
93 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0336 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0395 (20°C, supercooled liquid, Murphy et al. 1987)
0.0221 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00803 (GC-RI correlation, Burkhard et al. 1985b)
0.00487, 0.00667 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.32×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 10.90 - 4650/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0038, 0.00589(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4399/(T/K) + 12.44$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
73.16 (calculated-P/C, Burkhard 1984)
27.46 (20°C, calculated-P/C, Murphy et al. 1987)
35.78 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
12.16 (wetted-wall column-GC/ECD, Brunner et al. 1990)
35.05 (calculated-QSPR, Dunnivant et al. 1992)
9.03 (calculated-QSPR, Achman et al. 1993)
42.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
54.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 10 \pm 5$ kJ/mol, $\Delta S_H = 0.00 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.31 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
6.31 (calculated-TSA, Burkhard 1984)

5.87 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.87 (recommended, Sangster 1993)
5.9623 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.07 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

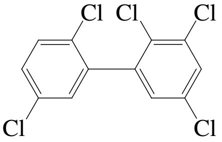
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.11 (suspended particulate matter, Burkhard 1984)
4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 10 (food lipid mg)/(g worm lipid-d); k_2 = 0.08 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.08 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{½}$ = 166 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{½}$ = 217 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 8 d in earthworm given contaminated food (Wågman et al. 2001)
depuration $t_{½}$ = 166 d for high-dose treatment, $t_{½}$ = 217 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.92 2,2′,3,5,5′-Pentachlorobiphenyl (PCB-92)



Common Name: 2,2′,3,5,5′-Pentachlorobiphenyl
Synonym: PCB-92, 2,2′,3,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5,5′-pentachlorobiphenyl
CAS Registry No: 52663-61-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
53 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0379 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00494 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.92×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00422, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00394, 0.00458 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P/\text{mmHg}) = 11.0 - 4740/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00302, 0.00447 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4522/(T/K) + 12.76$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
33.64 (calculated-P/C, Burkhard 1984)
32.63 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
26.35 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
28.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
48.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 6$ kJ/mol, $\Delta S_H = 0.05 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.05, 6.97 (RP-HPLC-k′ correlation:uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.32 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.11 (generator column-GC, Larsen et al. 1992)
6.32 (recommended, Sangster 1993)
6.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

8.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.11 (suspended particulate matter, Burkhard 1984)

4.726 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.005 d^{-1} with $t_{½}$ = 135 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 141 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

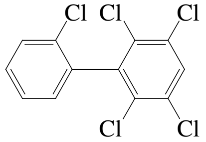
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 135 d for high-dose treatment, $t_{½}$ = 141 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.93 2,2′,3,5,6-Pentachlorobiphenyl (PCB-93)



Common Name: 2,2′,3,5,6-Pentachlorobiphenyl
Synonym: PCB-93, 2,2′,3,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5,6-pentachlorobiphenyl
CAS Registry No: 73575-56-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
91 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0411 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0149, 0.0164, 0.00986, 0.0119 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0151 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.0160, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00708 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4399/(T/K) + 12.57$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
120.6 (calculated-P/C, Burkhard 1984)
28.78 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
34.49 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)
5.99, 6.06, 6.07, 6.12 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.06 (recommended, Sangster 1993)
6.1176 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.09	(suspended particulate matter, Burkhard 1984)
4.611	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

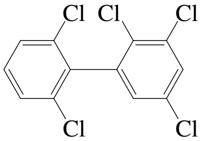
Ground water:

Sediment:

Soil:

Biota:

7.1.1.94 2,2′,3,5,6′-Pentachlorobiphenyl (PCB-94)



Common Name: 2,2′,3,5,6′-Pentachlorobiphenyl
Synonym: PCB-94
Chemical Name: 2,2′,3,5,6′-pentachlorobiphenyl
CAS Registry No: 73575-55-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):

79	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

289.1	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0336	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0259	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):

7.24×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00774, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

70.62	(calculated-P/C, Burkhard 1984)
43.98	(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
39.69	(calculated-QSPR, Dunnivant et al. 1992)
51.2	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.36	(calculated-TSA, Burkhard 1984)
6.13	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0371	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

8.64	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.16	(suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

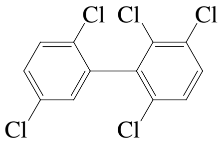
Ground water:

Sediment:

Soil:

Biota:

7.1.1.95 2,2′,3,5′,6-Pentachlorobiphenyl (PCB-95)



Common Name: 2,2′,3,5′,6-Pentachlorobiphenyl
Synonym: PCB-95, 2,2′,3,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5′,6-pentachlorobiphenyl
CAS Registry No: 38379-99-6
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
98.5–100 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.184 (mp at 100°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0336 (supercooled liquid S_L, calculated-TSA, Burkhard 1985b)
0.0541 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0291, 0.0216, 0.0192, 0.0156; 0.021 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0259 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011 (calculated-MCI χ, Patil 1991)
0.00190 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00735, 0.00905, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00849 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00537, 0.00744 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00335 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/mmHg) = 10.90 - 4650/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00427, 0.00741 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4399/(T/K) + 12.48$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
0.00295 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994; Harner & Bidleman 1996)
0.00211 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C):
82.78 (calculated-P/C, Burkhard 1985b)
20.06 (20°C, calculated-P/C, Murphy et al. 1987)
29.38 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
30.39 (calculated-QSPR, Dunnivant et al. 1992)
30.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 21 \pm 5$ kJ/mol, $\Delta S_H = 0.04 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.18 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
5.67, 5.98, 5.86, 6.05 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.08 (generator column-GC, Larsen et al. 1992)
5.92 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

9.06 (20°C, generator column-GC, measured range – 10 to 30°C, Harner & Bidleman 1996)
10.51, 9.06, 9.51, 9.06, 8.55 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
log $K_{OA} = -4.30 + 3904/(T/K)$; temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log $K_{OA} = -5.84 + 4360/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.80 (quoted, Kömp & McLachlan 1997b, Kaupp & McLachlan 1999)
10.07, 9.06; 9.07 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.04 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.3–6.8, 6.1; 7.40 (suspended sediment, average; algae > 50 µm, Oliver 1987a)
6.30 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.60, 4.66, 4.61, 3.70 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
4.603, 4.589 (marine humic substances, observed; calculated-MCI χ, reported as association coefficient log K_h at 5 mg/L DOC, Sabljic et al. 1989)
5.68, 5.70, 5.64 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.55 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.00030\ h^{-1}$; $k_2 = 0.184\ h^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 164$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003\ d^{-1}$ with $t_{½} = 225$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{1/2}$ = 8.29 min when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

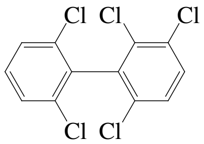
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 164 d for high-dose treatment, $t_{1/2}$ = 225 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.96 2,2′,3,6,6′-Pentachlorobiphenyl (PCB-96)



Common Name: 2,2′,3,6,6′-Pentachlorobiphenyl
Synonym: PCB-96
Chemical Name: 2,2′,3,6,6′-pentachlorobiphenyl
CAS Registry No: 73575-54-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
53 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0368 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0157 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00166, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
139.8 (calculated-P/C, Burkhard 1984)
38.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
41.56 (calculated-QSPR, Dunnivant et al. 1992)
62.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 15 \pm 3$ kJ/mol, $\Delta S_H = 0.02 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.33 (calculated-TSA, Burkhard 1984)
5.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.5365 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:
8.77 (20°C, generator column-GC/ECD, measured range –10 to 30°C, Harner & Bidleman 1996)
10.28, 9.72, 9.22, 8.77, 8.30 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
$\log K_{OA} = -4.60 + 3913/(T/K)$, temp range –10 to 30°C (Harner & Bidleman 1996)
9.87, 8.79; 8.76 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.82 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.13 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

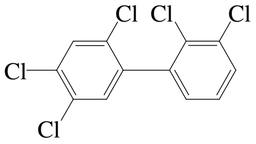
Ground water:

Sediment:

Soil:

Biota:

7.1.1.97 2,2′,3,4′,5′-Pentachlorobiphenyl (PCB-97)



Common Name: 2,2′,3,4′,5′-Pentachloro
Synonym: PCB-97
Chemical Name: 2,2′,3′,4,5-pentachlorobiphenyl
CAS Registry No: 41464-51-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
82 (Burkhard et al. 1984b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.77 (quoted, Shiu & Mackay 1986)
Fugacity Ratio at 25°C, F:
0.279 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0431 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0284 (20°C, supercooled liquid, Murphy et al. 1987)
0.00622, 0.00651, 0.00383, 0.00682 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0099 (literature average, Paya-Perez et al. 1991)
0.00847 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.01×10^{-3}, 8.05×10^{-4}, 8.04×10^{-4} (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00251, 0.00265 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.31×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/mmHg) = 11.10 - 4790/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
1.85×10^{-3}, 2.88×10^{-3} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.56$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0026 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
20.67 (calculated-P/C, Burkhard 1984)
15.1 (20°C, calculated-P/C, Murphy et al. 1987)
18.14 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
7.50 (wetted-wall column-GC/ECD, Brunner et al. 1990)
18.23 (calculated-QSPR, Dunnivant et al. 1992)

23.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
45.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 6$ kJ/mol, $\Delta S_H = 0.07 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.75, 6.67 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.25, 6.33, 6.35, 6.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.31 (recommended, Sangster 1993)
6.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
10.49, 9.44 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.21 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:
5.43; 6.96 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.40, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.40, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
6.07 (suspended particulate matter, Burkhard 1984)
4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)
5.83, 5.89, 5.78 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.69 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
6.10 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 3400 d^{-1}; k_2 = 0.0126 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{½}$ = 163 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 188 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

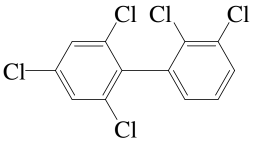
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 163 d for high-dose treatment, $t_{½}$ = 188 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.98 2,2′,3,4′,6′-Pentachlorobiphenyl (PCB-98)



Common Name: 2,2′,3,4′,6′-Pentachlorobiphenyl
Synonym: PCB-98
Chemical Name: 2,2′,3,4′,6′-pentachlorobiphenyl
CAS Registry No: 60233-25-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
93 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0333 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0153, 0.0116, 0.0124 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.05×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00753, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00615, 0.00751 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00692 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4399/(T/\text{K}) + 12.54$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
68.90 (calculated-P/C, Burkhard 1984)
50.26 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
39.69 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.36 (calculated-TSA, Burkhard 1984)
5.98, 6.16, 5.99 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.071 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, Burkhard 1984)

4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.005 d^{-1} with $t_{½}$ = 153 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

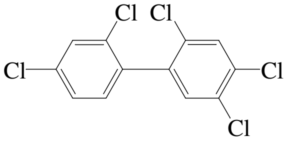
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 153 d for high-dose treatment, $t_{½}$ = 164 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.99 2,2′,4,4′,5-Pentachlorobiphenyl (PCB-99)



Common Name: 2,2′,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-99, 2,2′,4,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,5-pentachlorobiphenyl
CAS Registry No: 38380-01-7
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
81.0 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0353 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0222 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00366 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0103 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011 (calculated-MCI χ, Patil 1991)
0.00597 (estimated-EPIWIN v3.04, Hardy 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0029 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.00735, 0.00342, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00316 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.00328, 0.00375 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00147 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/mmHg) = 11.0 - 4740/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0024, 0.00347 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4533/(T/K) + 12.68$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
0.00229 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.000293 (estimated-EPIWIN v3.04, Hardy 2002)

Henry's Law Constant (Pa m^3/mol at 25°C):
29.28 (calculated-P/C, Burkhard et al. 1985b)
21.68 (20°C, calculated-P/C, Murphy et al. 1987)
30.50 (calculated-QSAR MCI χ, Sabljic & Güsten 1989)
7.90 (wetted-wall column-GC/ECD, Brunner et al. 1990)
57.0 (calculated-QSPR, Dunnivant et al. 1992)
9.39 (estimated-bond method EPIWIN v3.04, Hardy 2002)
35.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
51.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 16 \pm 6$ kJ/mol, $\Delta S_H = 0.02 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.29, 7.21 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.41 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
6.39 (calculated-TSA, Hawker & Connell 1988a)
6.26 (calculated-MCI χ, Patil 1991)
6.41 (recommended; Sangster 1993)
7.21 (recommended, Hansch et al. 1995)
6.60, 6.26–7.21 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
6.4014 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.9795 (estimated-EPIWIN v3.04, Hardy 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.38 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.09 (fish, microcosm, Garten & Trabalka 1983)
5.14 (estimated-EPIWIN v3.04, Hardy 2002)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.70, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:

6.14 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.73 (marine humic substance, calculated-MCI χ, reported as log K_h at 5 mg /L DOC, Sabljic et al. 1989)
7.00 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.68 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.54 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
6.10 (soil, calculated-K_{OW}, Girvin & Scott 1997)
4.87 (estimated-EPIWIN v3.04, Hardy 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 0.6419 d from river, $t_{1/2}$ = 13.31 d from lake (estimated-EPIWIN v3.04, Hardy 2002).

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 8 (food lipid mg)/(g worm lipid-d); k_2 = 0.07 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.003 d^{-1} with $t_{1/2}$ = 2252 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{1/2}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: volatilization $t_{1/2}$ = 0.6419 d from river, $t_{1/2}$ = 13.31 d from lake (estimated-EPIWIN v.3.04, Hardy 2002).

Groundwater:

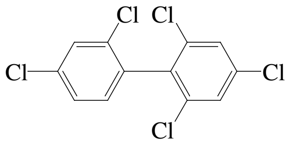
Sediment:

Soil:

Biota: elimination $t_{1/2}$ = 9 d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2}$ = 252 d for high-dose treatment, $t_{1/2}$ = 172 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.100 2,2′,4,4′,6-Pentachlorobiphenyl (PCB-100)



Common Name: 2,2′,4,4′,6-Pentachlorobiphenyl
Synonym: PCB-100, 2,2′,4,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,6-pentachlorobiphenyl
CAS Registry No: 39485-83-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
95 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0275 (supercooled liq. S_L, calculated-TSA, Burkhard et al. 1985b)
0.031 (unpublished data of Weil 1978; quoted, Kilzer et al. 1979; Geyer et al. 1980)
0.00666, 0.00580, 0.00941 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.011 (calculated-MCI χ, Patil 1991)
0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.00735, 0.00872, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al 1985a)
0.00818 (supercooled liquid, GC-RT correlation, Burkhard et al. 1985b; quoted, Eisenreich 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
97.27 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
62.62 (calculated-MCI χ, Sabljic & Güsten 1989)
56.98 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.23, 6.37, 6.08 (RP-HPLC-RI correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.23 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:
8.66 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
1.11, 1.06 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
0.32 (rodent, Garten & Trabalka 1983)
4.06, 3.91 (algae, calculated, Geyer et al. 1984)
4.06, 3.37, 4.44 (algae, fish, activated sludge, Freitag et al. 1984,1985; quoted, Halfon & Reggiani 1986)

Sorption Partition Coefficient, log K_{OC}:

6.24	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.567	(marine humic substance, calculated-MCI χ, reported as association coefficient log K_h at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.010 d^{-1} (10°C, sandworm, Goerke & Ernst 1977; quoted, Waid 1986)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

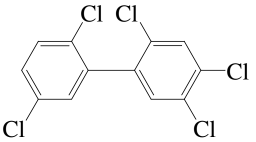
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.101 2,2′,4,5,5′-Pentachlorobiphenyl (PCB-101)



Common Name: 2,2′,4,5,5′-Pentachlorobiphenyl
Synonym: PCB-101, 2,2′,4,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5,5′-pentachlorobiphenyl
CAS Registry No: 37680-72-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
78.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2803
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
18.8 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.56 (Miller et al. 1984)
53.7, 65.6 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C, F:
0.318 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)
0.0321 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.031 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.0103 (shake flask-GC/ECD, Haque & Schmedding 1975; Chiou et al. 1977)
0.0042 (generator column-GC/ECD, Weil et al. 1974)
0.019 (shake flask-LSC, Metcalf et al. 1975)
0.010 (24°C, shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977)
0.00424 (16.5°C, shake flask-GC/ECD, Wiese & Griffin 1978)
0.0005; 0.004 (generator column-HPLC/UV; RP-HPLC-RT correlation, Swann et al. 1983)
0.0194 (generator column-GC/ECD, Miller et al. 1984, 1985)
0.0356 (supercooled liquid P_L, calculated-TSA, Burkhard et al. 1985b)
0.0154* (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
$\ln x = -3837/(T/K) - 8.0159$, temp range 4–32°C, ΔH_{ss} = 31.9 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
$\log x = -1664/(T/K) - 3.478$, ΔH_{ss} = 31.8 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
$S/(mol/L) = 1.54 \times 10^{-10} \exp(0.046 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
0.011 (shake flask-GC/ECD, Chiou et al. 1986, 1991)
0.0263 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00402, 0.00517, 0.0070, 0.0070 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00674; 0.0222(generator column-GC/ECD, supercooled liquid S_L, Dunnivant & Elzerman 1988)
$\log [S_L/(mol/L)] = 0.875 - 982.6/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
$\ln x = -8.026 - 3836.44/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

0.0334 (calculated-mp and K_{OW}, Ran et al. 2002)
0.0312, 0.0333 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log S_L/(mol m^{-3}) = – 1113/(T/K) – 0.27 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0016 (P_S from GC-RT correlation, Westcott & Bidleman 1981)
0.00096, 0.00173 (solid P_S: 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
log (P/mmHg) = 11.1 – 4840/(T/K); temp range 30–40°C (gas saturation-GC, Westcott et al. 1981)
0.0031 (P_L calculated from P_S using fugacity ratio F, Westcott & Bidleman 1981)
0.0053, 0.00316 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.00315 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
0.00336, 0.00402 (supercooled liquid P_L, calculated from P_{GC}, GC-RT correlation, different stationary phases, Bidleman 1984)
0.00358 (supercooled liquid P_L, GC-RT correlation, Burkhard 1984, Burkhard et al. 1985b)
0.00225, 0.00118, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00361, 0.00403 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00109; 0.0035 (selected solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
0.00142 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00359 (supercooled liquid P_L, Dunnivant & Elzerman 1988)
0.000527; 0.00173 (calculated-S × HLC, solid P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
log (P/mmHg) = 11.0 – 4750/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00152 (calculated-UNIFAC group contribution, Banerjee et al. 1990)
0.00315, 0.00296 (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.00504, 0.0034 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (P_L/Pa) = 12.13 – 4369/(T/K) (GC-RT correlation, Hinckley et al. 1990)
0.00257, 0.00398 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4514/(T/K) + 12.67 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
1.86×10^{-3} (supercooled liquid P_L, 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
1.33×10^{-4}, 4.16×10^{-4} (solid, supercooled liquid, Passivirta et al. 1999)
log (P_S/ Pa) = 15.47 – 5495/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 12.67 – 4514/(T/K) (liquid, Passivirta et al. 1999)
$(4.04–22.5) \times 10^{-4}$; $(1.46–40.4) \times 10^{-3}$ (literature solid P_S range; literature liquid P_L range, Delle Site 1997)
0.0020 (supercooled P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.0024, 0.00245 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = – 4632/(T/K) + 12.92 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log P_L/Pa = – 4346/(T/K) + 11.94 (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
11.46–35.46 (calculated-P/C, Westcott et al. 1981)
32.73 (calculated-P/C, Burkhard et al. 1985b)
7.09 (20°C, gas stripping-GC, Oliver 1985)
35.48 (calculated-P/C, Shiu & Mackay 1986)
18.14 (20°C, calculated-P/C, Murphy et al. 1987)
25.43 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
47.19 (calculated-QSAR-χ, Sabljic & Güsten 1989)
9.12 (wetted-wall column-GC/ECD, Brunner et al. 1990)
24.87 (calculated-QSPR, Dunnivant et al. 1992)
1.424, 4.166 (0, 15°C, from modified two-film model, Hornbuckle et al. 1994)
log H (Pa m^3/mol) = 13.55 – 3531/(T/K) (Passivirta et al. 1999)
42.07* ± 0.70 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
ln K_{AW} = 7.9384 – 3572.29/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(29.7/\text{kJ·mol}^{-1})/RT + (0.066/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 $J·K^{-1}·mol^{-1}$ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)

43.2 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
31.62, 24.0 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 3233/(T/K) + 12.21 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
4.12 (radiolabeled-^{14}C, Metcalf et al. 1975)
6.11 (shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977; Chiou et al. 1982)
7.64 (Hansch & Leo 1979)
6.44 (HPLC-RT correlation, Veith et al. 1979)
6.85 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.42 (HPLC-RT correlation, Swann et al. 1983)
5.92 (generator column-GC/ECD, Miller et al. 1984)
6.15, 7.07 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
7.64 (HPLC-RT correlation, Woodburn et al. 1984)
6.50 (generator column-HPLC, Woodburn et al. 1984)
6.88, 7.0 (HPLC-k′ correlation, calculated, De Kock & Lord 1987)
6.50 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
6.36, 6.39, 6.18, 6.27 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.88 (HPLC-RT correlation, Doucette & Andren 1988)
6.23, 6.18 (RP-HPLC-k′ correlation, different stationary phases, Sherblom & Eganhouse 1988)
6.41 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.16 (recommended, Sangster 1993)
6.50 (recommended, Hansch et al. 1995)
6.15, 6.33 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.
8.30 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
9.31* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = – 3.82 + 3841/(T/K); temp range –10 to 30°C (generator Column-GC, Harner & Bidleman 1996)
8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = – 5.84 + 4360/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
9.79 (10°C, estimated, Thomas et al. 1998)
10.49, 9.44; 9.29 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.37 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.14; 9.05 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.90, 8.73 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4291/(T/K) – 5.50 (LDV linear regression of literature data, Li et al. 2003)
log K_{OA} = 3785/(T/K) – 5.35 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
3.18 (green sunfish, 15 d in static water, Sanborn et al. 1975)
3.74, 4.78, 4.08, 4.24 (algae, snail, fish, mosquito, Metcalf et al. 1975)
4.66 (fish, flowing water, Kenaga & Goring; Kenaga 1980)
3.92, 3.60 (calculated-S, calculated-K_{OC}, Kenaga 1980)
4.09 (fish, microcosm, Garten & Trabalka 1983)
3.30–4.15 highest value, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
> 5.40, 4.15; 6.92 (rainbow trout, laboratory data: kinetic BCF; steady state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
2.73, 2.60 (human fat of lipid, wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
4.15 (fish, quoted, Isnard & Lambert 1988)

6.55 (rainbow trout, lipid basis, Noegrohati & Hammers 1992)
5.47; 7.00 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
3.32–5.15 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.84–6.26 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.06, 6.06 (*Daphnia*, 21-d renewal: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.47, 7.0 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.10, 7.02 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.03; 3.98 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:
4.63 (Kenaga & Goring 1980)
4.74, 4.80 (estimated-S, K_{OW}, Lyman 1982)
5.13, 4.67 (estimated-BCF, Lyman 1982)
4.70; 5.45 (soil, slurry method; HPLC-RT correlation, Swann et al. 1983)
6.14 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.60; 5.50; 6.60 (field data of sediment trap material; Niagara River-organic matter; calculated-K_{OW}, Oliver & Charlton 1984)
5.65 (suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
6.68, 5.58 (suspended solids-Lake Superior: calculated-K_{OW}, Baker et al. 1986)
4.87, 4.07 (Sanhedron soil, Suwannee River, humic acid, shake flask-GC/ECD, Chiou et al. 1986,1987)
4.12, 4.10 (Sanhedron soil, Suwannee River, fulvic acid, shake flask-GC/ECD, Chiou et al. 1986,1987)
5.1–6.7, 6.2 (suspended sediment, average, Oliver 1987a)
5.41, 5.41, 4.81, 4.09, 4.01 (Aldrich humic acid Na salt, Fluka-Tridon humic acid, Calcasieu River humic extract, Suwannee River water sample, Sopchoppy River water sample, Chiou et al. 1987)
6.25 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.77, 4.86, 4.80, 3.86 (humic substances, in concentrations. of 5, 10, 20, 40 mg C/L, reported as log K_h, Lara & Ernst 1989)
4.772, 4.726 (marine humic substances of 5 mg/L DOC, reported as association coefficient log K_h, quoted exptl; calculated-MCI χ, Sabljic et al. 1989)
5.86 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.58 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.81, 5.83, 5.78 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.67 (soil, shake flask-GC, Paya-Perez et al. 1991)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.63 (soil, Sabljic et al. 1995)
5.80; 5.58 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.90; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
5.73 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)
4.78–7.03; 4.60–6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.59; 6.19, 5.53, 6.04 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log K_{OM}:
4.63, 4.84 (quoted, calculated-molecular connectivity indices χ, Sabljic 1984)

Sorption Partition Coefficient, log K_P:
4.87–5.35 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photodegradation rate constants k = (0.20 ± 0.01) h^{-1}, (0.20 ± 0.04) h^{-1}, with $t_{½}$ = 3.4 h, 3.7 h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 4.6 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: degradation rate, k = 1.5 × 10^{-8} nmol $cell^{-1}$ h^{-1} by species of Alcaligenes and Acinetobacter (Furukawa et al. 1978, selected, NAS 1979);

85% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986);

aerobic biodegradation $t_{½}$ = 1.32 d with the addition of polymer chitin, $t_{½}$ = 0.80 d with chitin plus adapted microbes in flow microcosm with water and sedimentary materials from the field (Abramowicz 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 > 0.0007 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

k_1 = 180 d^{-1}; k_2 = 0.0007 d^{-1} (rainbow trout, Oliver & Niimi 1985)

k_1 = 0.049 h^{-1}; k_2 = 0.014 h^{-1} (mayfly-sediment model II, Gobas et al. 1989)

log 1/k_2 > 3.1, 3.6 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b).

k_1 = 3850 d^{-1}; k_2 = 0.0130 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.054 d^{-1} with an elimination $t_{½}$ = 12.9 d (earthworm, Belfroid et al. 1995)

k_2 = 0.005 d^{-1} with $t_{½}$ = 131 d and k_2 = 0.012 d^{-1} with $t_{½}$ = 56 d for food concn of 20 ng/g and 148 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_1 = 0.00082 h^{-1}; k_2 = 0.160 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)

k_1(calc) = 6 (food lipid mg)/(g worm lipid-d); k_2(calc) = 0.06 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.003 d^{-1} with $t_{½}$ = 246 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995);

suggested $t_{½}$ = 3000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: aerobic biodegradation $t_{½}$ = 1.32 d with the addition of polymer chitin, $t_{½}$ = 0.80 d with chitin plus adapted microbes in flow microcosm with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990);

half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);

photodegradation $t_{½}$ = (3.4 ± 015) h, (3.7 ± 0.8) h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995);

$t_{½}$ = 60000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.039 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.65 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.54 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.24 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are k = 0.00064 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00188 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00073 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00247 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

$t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{½}$ 1000 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{½}$ = 85 d in its muscle, (Niimi & Oliver 1983);

elimination $t_{½}$ = 12.9 from earthworm (Belfroid et al. 1995)

depuration $t_{½}$ = 56–131 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$t_{½}$ = 4.3 h in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination $t_{½}$ = 12 d in earthworm given contaminated food (predicted, Wågman et al. 2001).

depuration $t_{½}$ = 172 d for high-dose treatment, $t_{½}$ = 24446 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.101.1

Reported aqueous solubilities, vapor pressures, Henry's law constants and octanol-air partition coefficients of 2,2′,4,5,5′-pentachlorobiphenyl (PCB-101) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure		Henry's law constant		log K_{OA}	
Dickhut et al. 1986		Westcott et al. 1981		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas saturation-GC		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
4	0.0061	25	0.00096	4	15.75	–10	10.70
20	0.0121	30	0.00173	11	22.20	0	10.31
25	0.0154			18	30.78	10	9.78
32	0.0223			25	42.07	20	9.31
		log P/mmHg = A – B/(T/K)		31	54.40	30	8.78
ln x = A – B/(T/K)		A	11.1				
A	–8.0159	B	4840	ln K_{AW} = –ΔH/RT + ΔS/R		$ΔH_{OA}$/(kJ mol^{-1}) = 73.54	
B	3836.90	temp range 30–40°C		A	7.9384		
				B	3572.3	log K_{OA} = A + B/T	
$ΔH_{sol}$/(kJ mol^{-1}) = 31.9 ±1.9						A	–3.82
for 4–32°C				enthalpy, entropy change:		B	3841
				ΔH/(kJ·mol^{-1}) = 29.7 ± 3.2			
				ΔS/(J·mol^{-1}·K^{-1}) = 66 ± 10			

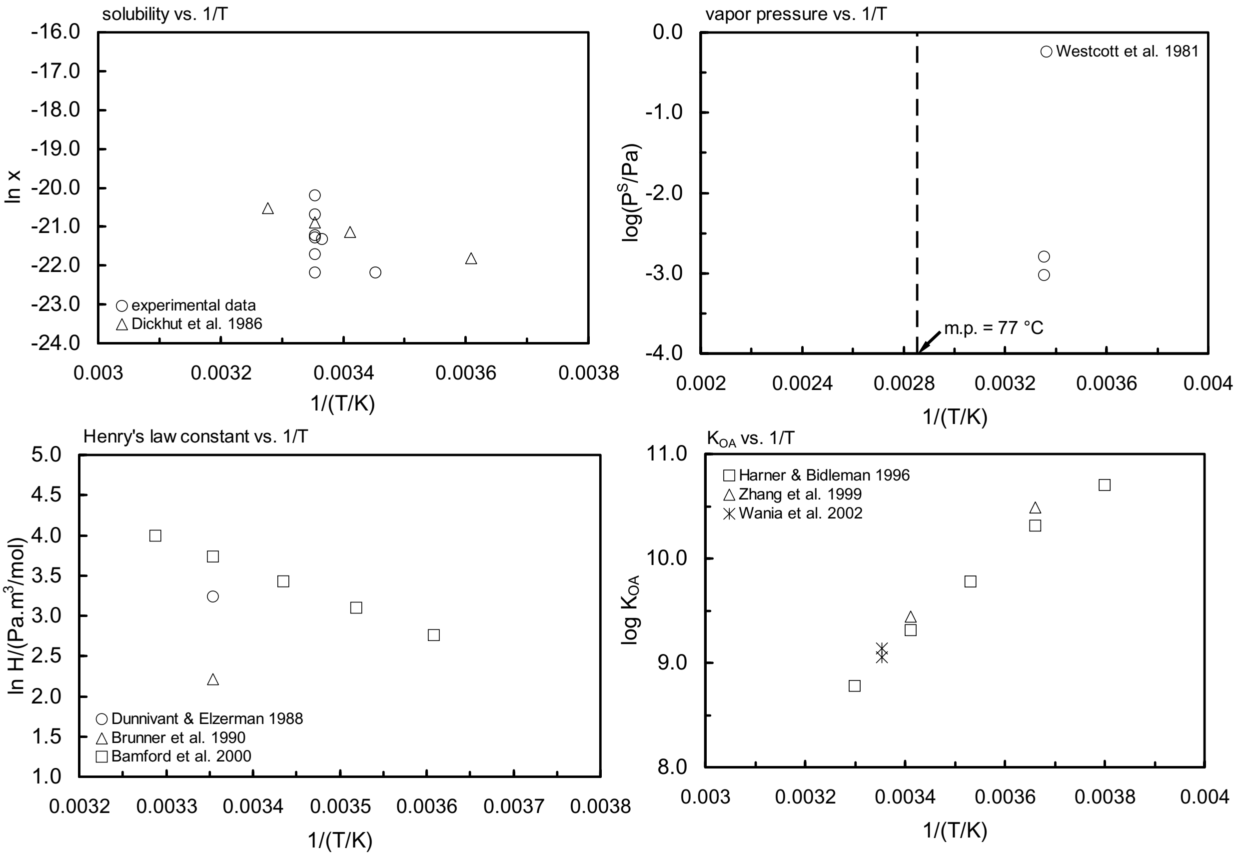
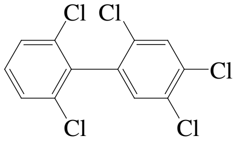


FIGURE 7.1.1.101.1 Logarithm of mole fraction solubility, vapor pressure, Henry's law constant and K_{OA} versus reciprocal temperature for 2,2′,4,5,5′-pentachlorobiphenyl (PCB-101).

7.1.1.102 2,2′,4,5,6′-Pentachlorobiphenyl (PCB-102)



Common Name: 2,2′,4,5,6′-Pentachlorobiphenyl
Synonym: PCB-102, 2,2′,4,5,6′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5,6′-pentachlorobiphenyl
CAS Registry No: 68194-06-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
93 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0314 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0065 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6.61×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00706, 0.00184 (calculated-MW, GC-RI correlation, calculated-χ, Burkhard et al. 1985b)
0.00527, 0.00667 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P/mmHg) = 10.80 - 4630/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
$\log (P_L/Pa) = -4399/(T/K) + 12.48$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
68.60 (calculated-P/C, Burkhard 1984)
35.26 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
9.12 (wetted-wall column-GC/ECD, Brunner et al. 1990)
37.6 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (calculated-TSA, Burkhard 1984)
6.16 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.0959 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.13 (calculated-QSPR/quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.19	(suspended particulate matter, Burkhard 1984)
4.589	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

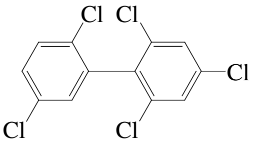
Ground water:

Sediment:

Soil:

Biota:

7.1.1.103 2,2′,4,5′,6-Pentachlorobiphenyl (PCB-103)



Common Name: 2,2′,4,5′,6-Pentachlorobiphenyl
Synonym: PCB-103, 2,2′,4,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5′,6-pentachlorobiphenyl
CAS Registry No: 60145-21-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
81 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0275 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00986, 0.00859, 0.0164, 0.0113 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.23×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00983, 0.00804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00887, 0.0112 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00617 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4399/(T/K) + 12.70$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
109.43 (calculated-P/C, Burkhard 1984)
56.24 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
51.02 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.44 (calculated-TSA, Burkhard 1984)
6.11, 6.25, 5.92, 6.14 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.22 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.11 (recommended, Sangster 1993)
8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.1499 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.00	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.24	(suspended particulate matter, Burkhard 1984)
4.567	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

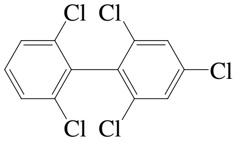
Ground water:

Sediment:

Soil:

Biota:

7.1.1.104 2,2′,4,6,6′-Pentachlorobiphenyl (PCB-104)



Common Name: 2,2′,4,6,6′-Pentachlorobiphenyl
Synonym: PCB-104, 2,2′,4,6,6′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,6,6′-pentachlorobiphenyl
CAS Registry No: 56558-16-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
85.0 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.258 (mp at 85°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.030 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0156 (generator column-GC, Dunnivant & Elzerman 1988)
0.0411 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.00986 (calculated-group contribution method, Kühne et al. 1995)
0.00651, 0.0175 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.0666 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C):
0.017 (supercooled liquid P_L, Burkhard 1984)
0.00735, 0.018, 0.00419 (supercooled liquid P_L, calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0170 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00434 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
0.00434 (calculated-S × HLC, solid P_S, Dunnivant & Elzerman 1988)
0.00225 (P_L, calculated-MCI ${}^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
185.4 (calculated-P/C, Burkhard et al. 1985b)
90.9 (gas stripping, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
55.4 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
75.11 (calculated-QSPR, Dunnivant et al. 1992)
39.40, 47.17, 56.0, 66.0* ± 1.4, 75.50 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 2.1650 - 1774.05/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(14.5/kJ{\cdot}mol^{-1})/\ RT] + (0.018/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where R = 8.314 $J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
62.0 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 15 ± 3 kJ/mol, ΔS_H = 0.02 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.40	(calculated-TSA, Burkhard 1984)
5.37	(generator column-GC, Hawker & Connell 1988a; quoted, Sangster 1993)
5.81	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
8.7057	(calculated-UNIFAC group contribution, Chen et al. 1993)
6.61	(calculated-Characteristic Root Index CRI, Saçan & Inel 1995)
5.7636	(calculated-molecular properties MNDO-AM1, Makino 1998)
5.96	(calculated-QSPR, Yeh & Hong 2002)
6.59	(calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

8.46	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.20	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.431	(marine humic substances, reported as association coefficient log K_h at 5 mg L^{-1} DOC, calculated-MCI χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 6$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.10$ d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

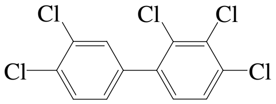
Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} > 1000$ d in rainbow trout, and $t_{1/2} = 101$ d in its muscle (Niimi & Oliver 1983);
elimination $t_{1/2} = 7$ d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.105 2,3,3′,4,4′-Pentachlorobiphenyl (PCB-105)



Common Name: 2,3,3′,4,4′-Pentachlorobiphenyl
Synonym: PCB-105, 2,3,3′,4,4′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′-pentachlorobiphenyl
CAS Registry No: 32598-14-4
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
103 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, assuming ΔS_{fus} = 56 J/mol K, F: 0.164 (at mp 103°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0405 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00236, 0.0119, 0.00636, 0.00517 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00206 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00190 (calculated-QSPR, Dunnivant et al. 1992)
0.000982, 0.00190(generator column-GC/ECD, estimated, Hong & Qiao 1995)
0.00166* (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.
0.0362, 0.08243(supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S_L/(mol m^{-3})] = – 1285/(T/K) + 0.18 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.7×10^{-4}, 9.35×10^{-4} (supercooled liquid P_L by GC-RT correlation, different stationary phases, Bidleman 1984)
7.07×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00124, 0.000132, 0.000233 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
8.85×10^{-4}, 6.77×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.62×10^{-4}, 7.76×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4758/(T/K) + 12.90 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
6.76×10^{-4} (supercooled liquid P_L, 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
2.54×10^{-3} (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)
8.71×10^{-4}, 1.23×10^{-3} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = – 4554/(T/K) + 12.29 (supercooled liquid P_L, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
5.68 (calculated-P/C, Burkhard 1985a)
6.08 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
10.06 (calculated-QSPR, Dunnivant et al. 1992)
2.43 (calculated-QSPR, Achman et al. 1993)

33.6* ± 1.3 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 26.221 - 9093.1/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(75.6/\text{kJ·mol}^{-1})/RT] + (0.218/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where $R = 8.314\ \text{J·K}^{-1}\text{·mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
33.9 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 76 \pm 8$ kJ/mol, $\Delta S_H = 0.22 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
33.88, 13.80 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log H/(\text{Pa m}^3/\text{mol}) = -3269/(T/K) + 12.1$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.41, 6.68, 7.14, 6.93 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.82 (generator column-GC; Hawker & Connell 1988a)
6.79 (recommended, Sangster 1993)
6.65 (recommended, Hansch et al. 1995)
4.97–5.10 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)
6.61 (generator column-GC/ECD, Yeh & Hong 2002)
6.61, 6.82 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
10.27* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
$\log K_{OA} = -5.68 + 4678/(T/K)$; (temp range –10 to 30°C, Harner & Bidleman 1996)
11.41, 10.20; 10.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.17 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.40, 7.34 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4630/(T/K) - 6.0$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF or log K_B:
2.82–4.26 (various marine species, mean dry weight, Hope et al. 1998)

Sorption Partition Coefficient, log K_{OC}:
6.09 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.906 (as log K_h, association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)
5.81 (soil, shake flask-GC, Paya-Perez et al. 1991)
6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48$ d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.014\ d^{-1}$ with $t_{½} = 48$ d and $k_2 = 0.014\ d^{-1}$ with $t_{½} = 50$ d for food concn of 17 ng/g and 133 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 181$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003\ d^{-1}$ with $t_{½} = 204$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment: $t_{½} = 7$ yr (Geyer et al. 2000)

Soil:

Biota: reported biological $t_{½} = 155$ to > 1000 d for trout, $t_{½} = 62–101$ d for trout muscle; $t_{½} = 73$ to > 200 d for carp for pentachlorobiphenyls (Niimi 1987)

Depuration $t_{½} = 49–50$ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{½} = 181$ d for high-dose treatment, $t_{½} = 204$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.105.1

Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,3,3′,4,4′-pentachlorobiphenyl (PCB 105) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
5	5.58×10^{-4}	4	3.09	–10	12.12
15	8.89×10^{-4}	11	7.10	0	11.43
25	1.66×10^{-3}	18	15.73	10	10.84
35	2.98×10^{-3}	25	33.6	20	10.27
		31	62.5	30	9.77
ln x = A – B/(T/K)					
mole fraction x		ln K_{AW} = –ΔH/RT + ΔS/R		$ΔH_{OA}$/(kJ mol^{-1}) = 89.57	
A		A	26.2208		
B	$ΔH_{sol}$/R	B	9093.1	log K_{OA} = A + B/T	
				A	–5.68
mp/°C	116.5–117.5	enthalpy, entropy change:		B	4678
$ΔH_{sol}$/(kJ mol^{-1}) = 40.1		ΔH/(kJ·mol^{-1}) = 75.6 ± 8.4			
		ΔS/(J·mol^{-1}·K^{-1}) = 218 ± 28			

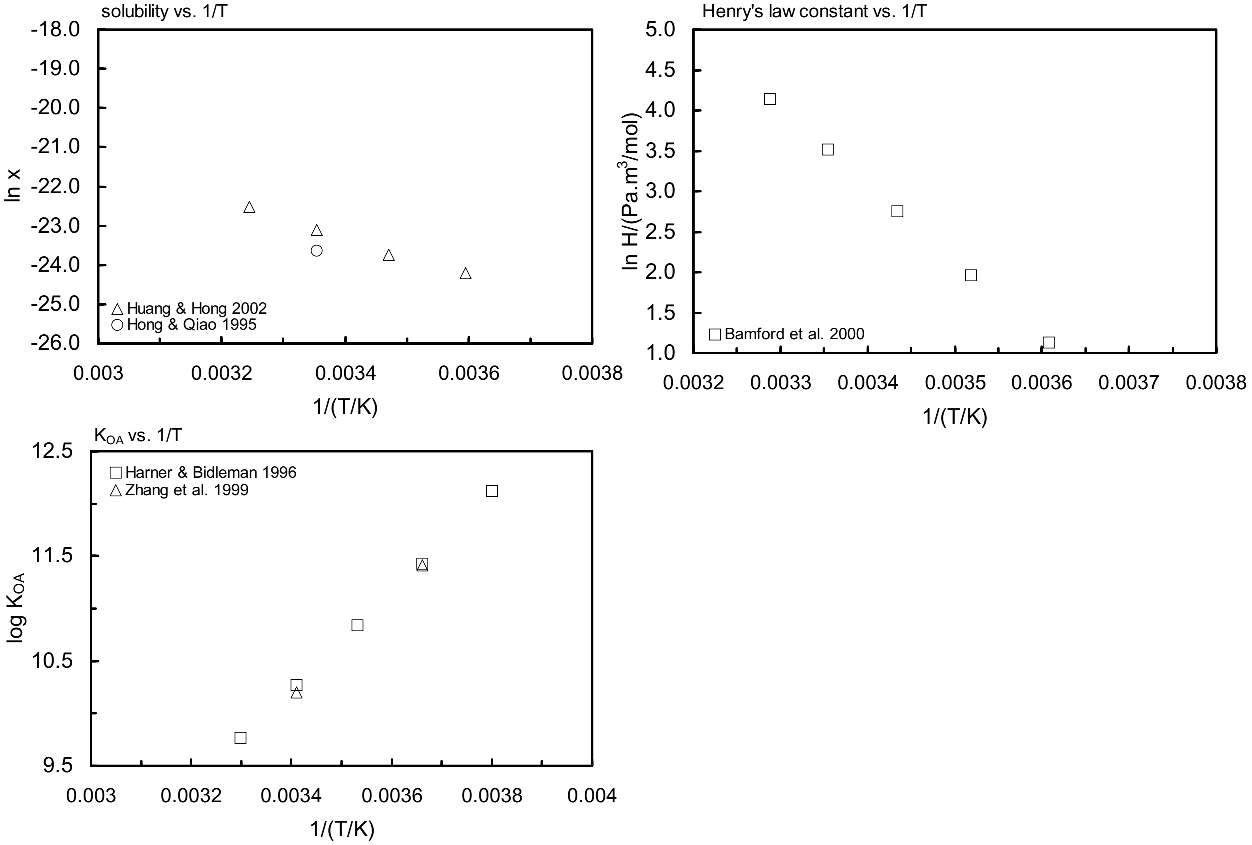
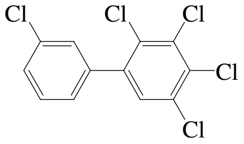


FIGURE 7.1.1.105.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,3,3′,4,4′-pentachlorobiphenyl (PCB-105).

7.1.1.106 2,3,3′,4,5-Pentachlorobiphenyl (PCB-106)



Common Name: 2,3,3′,4,5-Pentachlorobiphenyl
Synonym: PCB-106, 2,3,3′,4,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5-pentachlorobiphenyl
CAS Registry No: 70424-69-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
105 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0411 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0082, 0.0088, 0.00517, 0.0058 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00326 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0050 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.0180, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00138, 0.00127 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/\text{Pa}) = -4688/(T/K) + 12.86$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
39.82 (calculated-P/C, Burkhard 1984)
19.66 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
16.7 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)
6.79, 6.79, 7.22, 6.89 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.64 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.92 (recommended, Sangster 1993)
6.6213 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.09	(suspended particulate matter, Burkhard 1984)
4.906	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

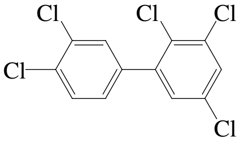
Ground water:

Sediment:

Soil:

Biota:

7.1.1.107 2,3,3′,4′,5-Pentachlorobiphenyl (PCB-107)



Common Name: 2,3,3′,4′,5-Pentachlorobiphenyl
Synonym: PCB-107, 2,3,3′,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5-pentachlorobiphenyl
CAS Registry No: 70424-68-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):

105	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

289.1	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0359	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0148	(20°C, supercooled liquid, Murphy et al. 1987)
0.0026	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.00105 (P_L supercooled liquid, Burkhard et al. 1985a)
0.00735, 0.00116, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
2.61×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
0.00105, 0.00132 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4688/(T/K) + 12.82$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

9.63	(calculated-P/C, Burkhard 1984)
8.61	(20°C, calculated-P/C, Murphy et al. 1987)
20.27	(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
16.13	(calculated-QSPR, Dunnivant et al. 1992)
3.94	(calculated-QSPR, Achman et al. 1993)
16.1	(11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.1	(from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 43 \pm 7$ kJ/mol, $\Delta S_H = 0.11 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.34	(calculated-TSA, Burkhard 1984)
6.71	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.5952	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.58	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.14	(suspended particulate matter, Burkhard 1984)
4.884	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{½}$ = 194 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.002 d^{-1} with $t_{½}$ = 283 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

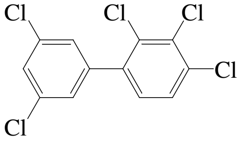
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 194 d for high-dose treatment, $t_{½}$ = 283 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.108 2,3,3′,4,5′-Pentachlorobiphenyl (PCB-108)



Common Name: 2,3,3′,4,5′-Pentachlorobiphenyl
Synonym: PCB-108, 2,3,3′,4,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5′-pentachlorobiphenyl
CAS Registry No: 70362-41-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
  73 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
  0.0356 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.0153 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  0.00517 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.00103 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.00735, 0.00115, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
  0.00142, 0.00118 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.00105 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
  $\log (P_L/Pa) = -4688/(T/K) + 12.87$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
  9.57 (calculated-P/C, Burkhard 1984)
  35.26 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  17.81 (calculated-QSPR, Dunnivant et al. 1992)
  36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 7$ kJ/mol, $\Delta S_H = 0.15 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  6.34 (calculated-TSA, Burkhard 1984)
  6.57 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  6.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
  6.6672 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
  9.86 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.14 (suspended particulate matter, Burkhard 1984)

4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

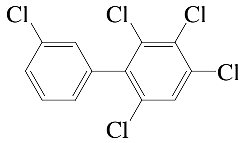
Ground water:

Sediment:

Soil:

Biota:

7.1.1.109 2,3,3′,4,6-Pentachlorobiphenyl (PCB-109)



Common Name: 2,3,3′,4,6-Pentachlorobiphenyl
Synonym: PCB-109, 2,3,3′,4,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,6-pentachlorobiphenyl
CAS Registry No: 74472-35-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
73 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0434 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0063 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00675, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
47.52 (calculated-P/C, Burkhard 1984)
28.56 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
39.42 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.27 (calculated-TSA, Burkhard 1984)
6.48 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.5063 (quoted exptl., calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.59 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.07 (suspended particulate matter, Burkhard 1984)
4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

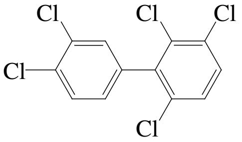
Ground water:

Sediment:

Soil:

Biota:

7.1.1.110 2,3,3′,4′,6-Pentachlorobiphenyl (PCB-110)



Common Name: 2,3,3′,4′,6-Pentachlorobiphenyl
Synonym: PCB-110, 2,3,3′,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,6-pentachlorobiphenyl
CAS Registry No: 38380-03-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
  79 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.0434 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
  0.0288 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  0.00731 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  0.0082 (calculated-TSA, Abramowitz & Yalkowsky 1990)
  0.011 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  0.00735, 0.00248, 0.000804(calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
  0.00228 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  0.00182, 0.00199(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  9.48×10^{-4} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  $\log (P/\text{mmHg}) = 11.0 - 4780/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
  0.00141, 0.00224 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
  $\log (P_L/\text{Pa}) = -4522/(T/K) + 12.43$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
  0.00258 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
  37.48 (calculated-P/C, Murphy et al. 1983)
  17.12 (calculated-P/C, Burkhard et al. 1985b)
  10.74 (20°C, calculated-P/C, Murphy et al. 1987)
  19.15 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  19.89 (calculated-QSPR, Dunnivant et al. 1992)
  5.966 (calculated-QSPR, Achman et al. 1993)
  18.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  42.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 38 \pm 7$ kJ/mol, $\Delta S_H = 0.09 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.20	(RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
6.48	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.22	(generator column-GC, Larsen et al. 1992)
6.20	(recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

9.06; 8.58 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log $K_{OA} = -6.16 + 4540/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
10.14 (10°C, estimated, Thomas et al. 1998)
9.06 (quoted, Kömp & McLachlan 1997b, Kaupp & McLachlan 1999)
10.61, 9.58; 9.80 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.19 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.18, 6.48 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.50 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:

6.06 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.6–6.8, 6.4; 7.70(suspended sediment, average; algae > 50μm, Oliver 1987a)
4.72, 4.80, 4.77, 3.79 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
4.72, 4.75 (marine humic substances of 5 mg/L DOC, quoted, calculated-MCI χ, Sabljic et al. 1989)
6.32 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.20 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.71 (soil, shake flask-GC, Paya-Perez et al. 1991)
6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.80 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodegradation rate constant $k = (0.07 \pm 0.01)\ h^{-1}$ with $t_{1/2} = 9.9$ h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.2–0.4) \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH\cdot}(aq.) = 4.3 \times 10^9\ dm^3\ mol^{-1}\ s^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(calc) = (0.3–0.9) \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.00064\ h^{-1}$; $k_2 = 0.094\ h^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 171$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003\ d^{-1}$ with $t_{1/2} = 204$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4$–11 d in freshwater systems, $t_{1/2} = 0.1$–10 d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

photodegradation $t_{1/2} = (9.9 \pm 1.6)$ h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

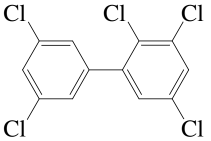
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 171$ d for high-dose treatment, $t_{1/2} = 204$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.111 2,3,3′,5,5′-Pentachlorobiphenyl (PCB-111)



Common Name: 2,3,3′,5,5′-Pentachlorobiphenyl
Synonym: PCB-111, 2,3,3′,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5,5′-pentachlorobiphenyl
CAS Registry No: 39635-32-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
79 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0315 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00411 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.00156 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00633, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
16.21 (calculated-P/C, Burkhard 1984)
49.45 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
19.89 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (calculated-TSA, Burkhard 1984)
6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.7224 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.08 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.19 (suspended particulate matter, Burkhard 1984)
4.862 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

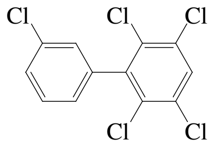
Ground water:

Sediment:

Soil:

Biota:

7.1.1.112 2,3,3′,5,6-Pentachlorobiphenyl (PCB-112)



Common Name: 2,3,3′,5,6-Pentachlorobiphenyl
Synonym: PCB-112, 2,3,3′,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5,6-pentachlorobiphenyl
CAS Registry No: 74472-36-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
 65 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
 289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
 0.0463 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
 0.00382, 0.00783, 0.00430, 0.00765 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
 5.91×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
 0.00735, 0.00633, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
 0.00316 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
 $\log (P_L/Pa) = -4522/(T/K) + 12.65$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
 41.75 (calculated-P/C, Burkhard 1984)
 33.34 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
 27.02 (calculated-QSPR, Dunnivant et al. 1992)
 44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
 6.24 (calculated-TSA, Burkhard 1984)
 6.40, 6.28, 6.70, 6.25 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 6.45 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
 6.41 (recommended, Sangster 1993)
 6.4916 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
 9.16 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.04	(suspended particulate matter, Burkhard 1984)
4.748	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 12 (food lipid mg)/(g worm lipid-d); k_2 = 0.06 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

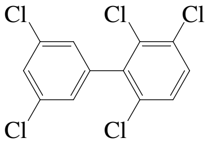
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2}$ = 11 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.113 2,3,3′,5′,6-Pentachlorobiphenyl (PCB-113)



Common Name: 2,3,3′,5′,6-Pentachlorobiphenyl
Synonym: PCB-113, 2,3,3′,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5′,6-pentachlorobiphenyl
CAS Registry No: 68194-10-5
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
65 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0382 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0036 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.372×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00365, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00306, 0.00368 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00240 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.63$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
28.88 (calculated-P/C, Burkhard 1984)
48.43 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
33.02 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.31 (calculated-TSA, Burkhard 1984)
6.45 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.54 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.45 (recommended, Sangster 1993)
6.3808 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.11 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm³ molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm³ molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: measured rate constant $k < 0.05$ M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.7–6.3 and 23 ± 2°C, with $t_{½} > 8$ d at pH 7 (Yao & Haag 1991).

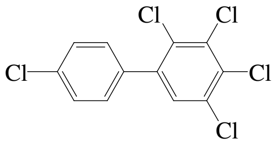
Ground water:

Sediment:

Soil:

Biota:

7.1.1.114 2,3,4,4′,5-Pentachlorobiphenyl (PCB-114)



Common Name: 2,3,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-114, 2,3,4,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′,5-pentachlorobiphenyl
CAS Registry No: 74472-37-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):

99	(Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
109	(Ruelle & Kesselring 1997)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

289.1	(calculated-Le Bas method at normal boiling point)
224.5	(Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.188 (at mp 99°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):

0.0121, 0.00879(RP-HPLC-k′ correlation, different mobile phases, Brodsky & Ballschmiter 1988)
0.00146; 0.00246(generator column-GC/ECD; estimated, Hong & Qiao 1995)
0.00263 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.
0.000732, 0.00157, 0.00263, 0.00505 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

5.58×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00136, 0.000881, 0.000352 (calculated-MW, GC-RI correlation, calculated-χ, Burkhard et al. 1985b)
3.45×10^{-4} (20°C, supercooled liquid P_L, Murphy et al. 1987)
0.00124, 0.000115(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
6.92×10^{-4} (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4688/(T/K) + 12.82$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

42.56	(calculated-P/C, Burkhard et al. 1985a)
6.99	(20°C, calcd-P/C, Murphy et al. 1987)
11.55	(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
14.48	(calculated-QSPR, Dunnivant et al. 1992)
4.96	(calculated-QSPR, Achman et al. 1993)
36.7	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.29	(calculated-TSA, Burkhard 1984)

6.45, 6.78	(RP-HPLC-k′ correlation, different mobile phases, Brodsky & Ballschmiter 1988)
6.65	(calculated, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.72	(recommended, Sangster 1993)
6.5879	(calculated-molecular properties MNDO-AM1, Makino 1998)
6.47	(generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.62	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.34, 6.65	(fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.09	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.906	(as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{1/2}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{1/2}$ = 187 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

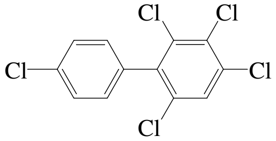
Sediment:

Soil:

Biota: reported biological $t_{1/2}$ = 155 to > 1000 d for trout, $t_{1/2}$ = 62–101 d for trout muscle; $t_{1/2}$ = 73 to > 200 d for carp for pentachlorobiphenyls (Niimi 1987)

depuration $t_{1/2}$ = 164 d for high-dose treatment, $t_{1/2}$ = 187 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.115 2,3,4,4′,6-Pentachlorobiphenyl (PCB-115)



Common Name: 2,3,4,4′,6-Pentachlorobiphenyl
Synonym: PCB-115, 2,3,4,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′,6-pentachlorobiphenyl
CAS Registry No: 74472-38-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
87 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0428 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00342, 0.00517, 0.00142, 0.00494 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0082 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.41×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00599, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00224 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4522/(T/K) + 12.50$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
42.56 (calculated-P/C, Burkhard 1984)
31.11 (calculated-QSAR- MCI χ, Sabljic & Güsten 1989)
24.87 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.27 (calculated-TSA, Burkhard 1984)
6.43, 6.40, 6.55, 6.38 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.49 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.44 (recommended, Sangster 1993)
6.4654 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.07	(suspended particulate matter, Burkhard 1984)
4.748	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 9 (food lipid mg)/(g worm lipid-d); k_2 = 0.07 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

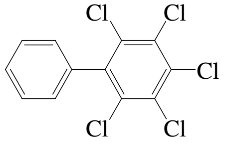
Ground water:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 11 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.116 2,3,4,5,6-Pentachlorobiphenyl (PCB-116)



Common Name: 2,3,4,5,6-Pentachlorobiphenyl
Synonym: PCB-116, 2,3,4,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4,5,6-pentachlorobiphenyl
CAS Registry No: 18259-05-7
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
123.5 (Lide 2003)
Boiling Point (°C):
381 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm^3 at 20°C): 1.2803
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.80 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
54.81 (Miller et al. 1984)
54.83, 65.6 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.108 (mp at 123.5°C)
0.105 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0068 (generator column-GC/ECD, Weil et al. 1974)
0.0207 (shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00548 (generator column-GC/ECD, Miller et al. 1984,1985)
0.00139, 0.00517, 0.00158, 0.00608 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00401 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0136 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.000788, 0.000394, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00341 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0024 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4522/(T/\text{K}) + 12.53$ (GC-RT correlation, Falconer & Bidleman 1994)
0.00326 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C):
18.34 (calculated-P/C, Burkhard et al. 1985b)
23.41 (calculated-QSPR-MCI χ, Sabljic et al. 1989)
29.97 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.85 (RP-TLC-retention time correlation, Bruggeman et al. 1982)
7.49 (calculated-f const., Yalkowsky et al. 1983)
6.30 (generator column-GC/ECD, Miller et al. 1984, 1985)
6.30; 6.70, 6.40, 6.65, 6.32 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.754 ± 0.015 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
6.25 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.52 (recommended, Sangster 1993)
6.74 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}

9.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Bioaccumulation Factor, log BAF:

5.46 (fish, lipid based-L/kg(lp), Thomann 1989)

Sorption Partition Coefficient, log K_{OC}:

5.94 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.791 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

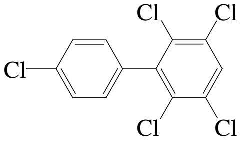
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm³ molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm³ molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2: > 0.0007 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ > 1000 d in rainbow trout, and $t_{½}$ = 100 d in its muscle, 100 d (Niimi & Oliver 1983).

7.1.1.117 2,3,4′,5,6-Pentachlorobiphenyl (PCB-117)



Common Name: 2,3,4′,5,6-Pentachlorobiphenyl
Synonym: PCB-117, 2,3,4′,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4′,5,6-pentachlorobiphenyl
CAS Registry No: 68194-11-6
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
115 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0457 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0042, 0.00651, 0.0248, 0.00494 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00411 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.23×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00561, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
$\log (P/\text{mmHg}) = 11.10 - 4800/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00257 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4522/(T/K) + 12.56$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
37.29 (calculated-P/C, Burkhard 1984)
25.13 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
33.02 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.25 (calculated-TSA, Burkhard 1984)
6.37, 6.33, 6.49, 6.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.46 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.39 (recommended, Sangster 1993)
6.4587 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.20 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.05 (suspended particulate matter, Burkhard 1984)

4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

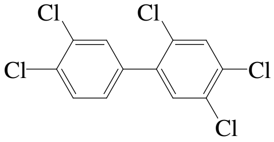
Ground water:

Sediment:

Soil:

Biota:

7.1.1.118 2,3′,4,4′,5-Pentachlorobiphenyl (PCB-118)



Common Name: 2,3′,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-118, 2,3′,4,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,5-pentachlorobiphenyl
CAS Registry No: 31508-00-6
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):

106	(Burkhard et al. 1985; Brodsky & Ballschmiter 1988)
109	(Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

289.1	(calculated-Le Bas method at normal boiling point)
224.5	(Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.158 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.01344 (20°C, supercooled liquid, Murphy et al. 1987)
0.0153 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00107; 0.00198 (generator column-GC/ECD; estimated, Hong & Qiao 1995)
0.00207* (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.
0.0290, 0.0223(supercooled liquid S_L: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S_L/(mol m^{-3})] = –1339/(T/K) + 0.32 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.00120 (P_L supercooled liquid, GC-RT correlation, Bidleman 1984)
9.62×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000167 (GC-RI correlation, Burkhard et al. 1985b)
0.00123, 0.00104 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.54×10^{-4} (20°C, supercooled liquid P_L, Murphy et al. 1987)
8.32×10^{-4}, 1.12×10^{-3} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4664/(T/K) + 12.72 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
8.91×10^{-4}, 1.0×10^{-4} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = –4853/(T/K) + 13.23 (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
log P_L/Pa = –4627/(T/K) + 12.52 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

40.8	(concn ratio-GC, Murphy et al. 1983)
8.61	(20°C, gas stripping-GC, Murphy et al. 1987)

11.75 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
3.94 (calculated-QSPR, Achman et al. 1993)
36.12* ± 1.0 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
ln K_{AW} = 15.877 – 5989.9/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(49.8/\text{kJ·mol}^{-1})/RT] + (0.132/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 $\text{J·K}^{-1}\text{·mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
36.3 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 50 ± 6 kJ/mol, ΔS_H = 0.13 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
32.36, 14.45 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log H/(Pa m^3/mol) = –2699/(T/K) + 10.56 (LDV linear regression of literature data, Li et al. 2003)
log H/(Pa m^3/mol) = –3289/(T/K) + 12.19 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
7.42 (HPLC-RT correlation, Shaw & Connell 1982)
6.66, 7.12 (HPLC-k′ correlation, Rapaport & Eisenreich 1984)
6.57 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.74 (calculated-TSA, Hawker & Connell 1988a)
6.24 (generator column-GC, Larsen et al. 1992)
6.57 (recommended, Sangster 1993)
6.49 (generator column-GC/ECD, Yeh & Hong 2002)
6.49, 6.69 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence. Additional data at other temperatures designated * are compiled at the end of this section:
10.08* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = –5.92 + 4693/(T/K); temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
11.13, 10.04; 10.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.86 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.80, 9.36 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4646/(T/K) – 6.22 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF or log K_B:
3.60–5.19 (various marine species, mean dry weight, Hope et al. 1998)
5.43 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)

Sorption Partition Coefficient, log K_{OC}:
6.16 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.88 (as log K_h, association coefficient with marine humic substance, calculated-χ, Sabljic et al. 1989)
5.81 (soil from Ispra near Lake Maggiore, Italy, batch equilibrium-GC/ECD, Paya-Perez et al. 1991)
5.20 (colloids and micro-particulates, GC/ECD, Murray & Andren 1992)
5.80 (calculated-K_{OW}, Girvin & Scott 1997)
5.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
4.79–7.42 (range, calculated from sequential desorption of 11 urban soils; Krauss & Wilcke 2001)
5.46; 6.03, 6.67, 6.26 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
6.16–7.20 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Sorption Partition Coefficient, log K_P of log K_d:
5.55–5.82 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)
5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.034 d^{-1} with an elimination $t_{½}$ = 20.3 d (earthworm, Belfroid et al. 1995)

k_2 = 0.007 d^{-1} with $t_{½}$ = 103 d and k_2 = 0.013 d^{-1} with $t_{½}$ = 53 d for food concn of 20 ng/g and 133 ng/g respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_1 = 14 L d^{-1} g^{-1} dry wt.; k_2 = 0.052 d^{-1} (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)

k_2 = 0.052 d^{-1} (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)

k_1 = 6 (food lipid mg)/(g worm lipid-d); k_2 = 0.06 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 180 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.003 d^{-1} with $t_{½}$ = 225 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: reported biological half-lives: $t_{½}$ = 155 to > 1000 d for trout, $t_{½}$ = 62–101 d for trout muscle; $t_{½}$ = 73 to > 200 d for carp for pentachlorobiphenyls (Niimi 1987);

elimination $t_{½}$ = 20.3 d from earthworm (Belfroid et al. 1995)

elimination $t_{½}$ = 95 d in rainbow trout, based on 228 d of elimination (Coristine et al. 1996)

depuration $t_{½}$ = 53–103 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

theoretical half-life to reach 90% steady-state tissue concn 13.3 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);

elimination $t_{½}$ = 12 d in earthworm given contaminated food (predicted, Wågman et al. 2001).

depuration $t_{½}$ = 180 d for high-dose treatment, $t_{½}$ = 225 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.118.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,3′,4,4′,5-pentachlorobiphenyl (PCB 118) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
5	5.85×10^{-4}	4	7.34	–10	11.93
15	1.22×10^{-3}	11	12.81	0	11.23
25	2.07×10^{-3}	18	21.79	10	10.64
35	3.31×10^{-3}	25	36.2	20	10.08
		31	54.8	30	9.57
ln x = A –B/(T/K)					
eq. 1	x	ln K_{AW} = –ΔH/RT + ΔS/R		ΔH_{OA}/(kJ mol^{-1}) = 89.86	
A		A	15.8768		
B	ΔH_{sol}/R	B	5989.9	log K_{OA} = A + B/T	
				A	–5.924
mp/°C	111–113	enthalpy, entropy change:		B	4693
ΔH_{sol}/(kJ mol^{-1}) = 37.4		ΔH/(kJ·mol^{-1}) = 49.8 ± 5.8			
		ΔS/(J·mol^{-1}·K^{-1}) = 132 ± 18			

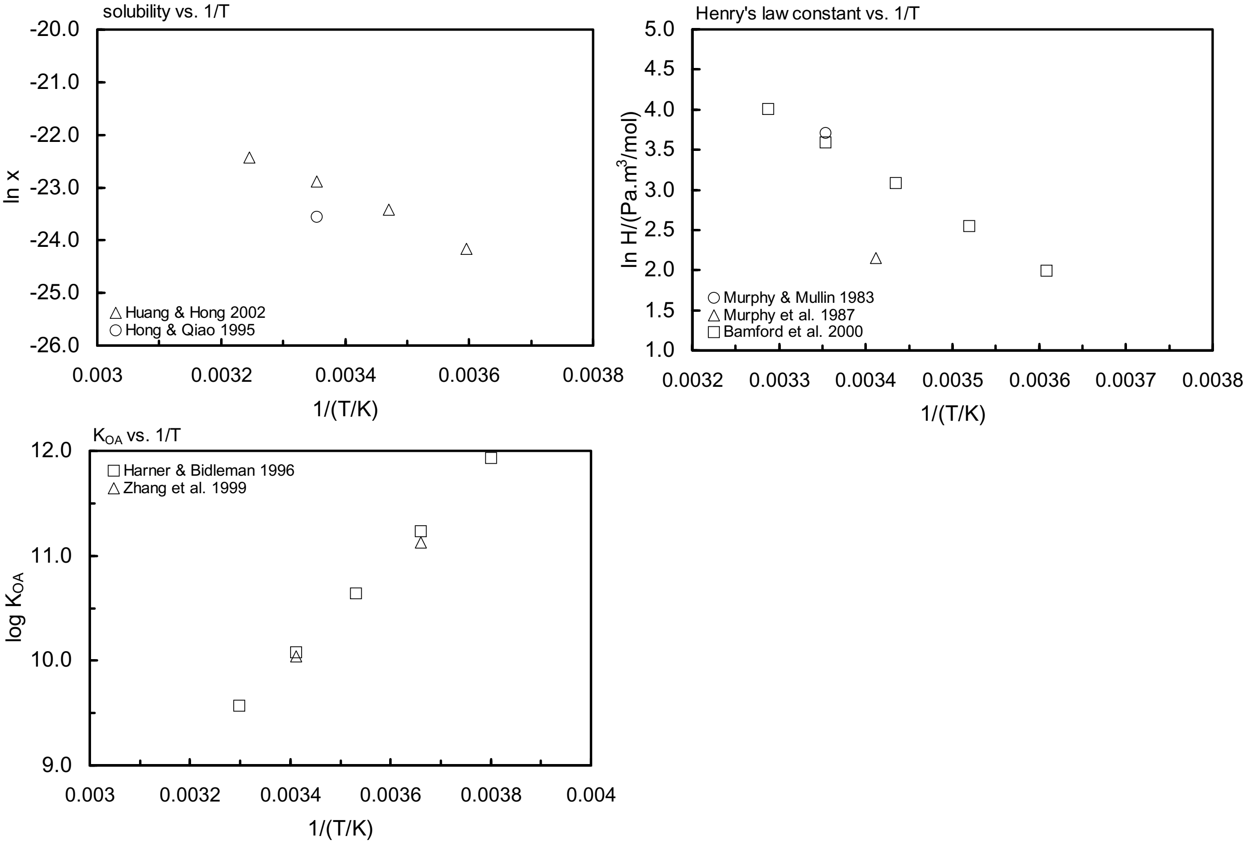
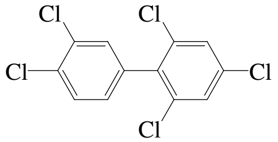


FIGURE 7.1.1.118.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,3′,4,4′,5-pentachlorobiphenyl (PCB-118).

7.1.1.119 2,3′,4,4′,6-Pentachlorobiphenyl (PCB-119)



Common Name: 2,3′,4,4′,6-Pentachlorobiphenyl
Synonym: PCB-119, 2,3′,4,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,6-pentachlorobiphenyl
CAS Registry No: 56558-17-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
  81 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
  0.0353 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.00326, 0.00375, 0.00411, 0.00529 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  0.00651 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  2.48×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)
  0.00735, 0.00269, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
  0.00288 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
  $\log (P_L/\text{Pa}) = -4522/(T/K) + 12.61$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
  22.90 (calculated-P/C, Burkhard 1984)
  46.10 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
  7.50 (wetted-wall column-GC/ECD, Brunner et al. 1990)
  5.97 (calculated-QSPR, Achman et al. 1993)
  31.46 (calculated-QSPR, Dunnivant et al. 1992)
  31.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  50.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 20 \pm 5$ kJ/mol, $\Delta S_H = 0.03 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  6.36 (calculated-TSA, Burkhard 1984)
  6.44, 6.49, 6.33, 6.35 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  6.58 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
  6.40 (recommended, Sangster 1993)
  8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)
  6.4124 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, Burkhard 1984)

4.726 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

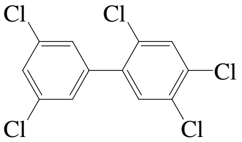
Ground water:

Sediment:

Soil:

Biota:

7.1.1.120 2,3′,4,5,5′-Pentachlorobiphenyl (PCB-120)



Common Name: 2,3′,4,5,5′-Pentachlorobiphenyl
Synonym: PCB-120, 2,3′,4,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,5,5′-pentachlorobiphenyl
CAS Registry No: 68194-12-7
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
77 (Shiu & Mackay 1986)
77, 93 (exptl., estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.306 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0295 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.42×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)
0.00735, 0.00155, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00197, 0.00203 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P/\text{mmHg}) = 11.0 - 4780/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
$\log (P_L/\text{Pa}) = -4688/(T/K) + 13.02$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
15.71 (calculated-P/C, Burkhard 1984)
40.94 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
6.57 (wetted wall column-GC/ECD, Brunner et al. 1990)
24.87 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.22, 5.68 (HPLC-k′ correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.41 (calculated-TSA, Burkhard 1984)
5.68 (quoted, Sangster 1993)
6.79 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.772 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.87	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.32	(suspended particulate matter, Burkhard 1984)
4.862	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

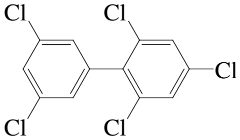
Ground water:

Sediment:

Soil:

Biota:

7.1.1.121 2,3′,4,5′,6-Pentachlorobiphenyl (PCB-121)



Common Name: 2,3′,4,5′,6-Pentachlorobiphenyl
Synonym: PCB-121, 2,3′,4,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,5′,6-pentachlorobiphenyl
CAS Registry No: 56558-18-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
91 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0311 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00201, 0.00259, 0.00651, 0.00682 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00411 (calculated-TSA and mp., Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.68×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00396, 0.000154 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00483, 0.00608(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00501 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4522/(T/\text{K}) + 12.85$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
38.50 (calculated-P/C, Burkhard 1984)
75.39 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
56.59 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (calculated-TSA, Burkhard 1984)
6.63, 6.60, 6.19, 6.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.64 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.42 (recommended, Sangster 1993)
6.5572 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.84 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.19	(suspended particular matter, Burkhard 1984)
4.704	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d for pentachlorobiphenyls (Atkinson 1987);
calculated tropospheric lifetime of 16–48 d for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

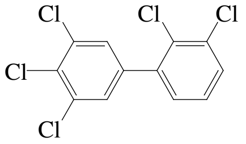
Ground water:

Sediment:

Soil:

Biota:

7.1.1.122 2,3,3′,4′,5′-Pentachlorobiphenyl (PCB-122)



Common Name: 2,3,3′,4′,5′-Pentachlorobiphenyl
Synonym: PCB-122
Chemical Name: 2,3,3′,4′,5′-pentachlorobiphenyl
CAS Registry No: 76842-07-4
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
111 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0128 (20°C, supercooled liquid, Murphy et al. 1987)
0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.76×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.000854, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
9.93×10^{-4}, 7.23×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.21×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P_L/\text{Pa}) = -4688/(T/\text{K}) + 12.72$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
6.21 (calculated-P/C, Burkhard 1984)
6.08 (20°C, calculated-P/C, Murphy et al. 1987)
13.88 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)
6.64 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.4986 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.09	(suspended particulate matter, Burkhard 1984)
4.906	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

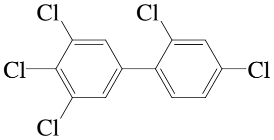
Ground water:

Sediment:

Soil:

Biota:

7.1.1.123 2,3′,4,4′,5′-Pentachlorobiphenyl (PCB-123)



Common Name: 2,3′,4,4′,5′-Pentachlorobiphenyl
Synonym: PCB-123, 2,3′,4,4′,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,5′-pentachlorobiphenyl
CAS Registry No: 65510-44-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
125 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.00201, 0.00259, 0.00651, 0.00682 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.000424 (generator column-GC/ECD, Hong & Qiao 1995)
0.000899 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by van Noort 2004.
0.000299, 0.000512, 0.000899, 0.00155 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.08×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00099 (P_L supercooled liquid values: GC-RI correlation, Burkhard et al. 1985b)
0.0013, 0.00095 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.000933 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4688/(T/K) + 12.84$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
8.805 (calculated-P/C, Burkhard 1984)
26.55 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
17.65 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.63, 6.60, 6.19, 6.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.74 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.64 (recommended, Sangster 1993)
6.4832 (calculated-molecular properties MNDO-AMI, Makino 1998)
6.50 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.83 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.884 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-χ, Sabljic et al. 1989)

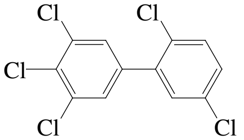
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 15–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water: photodegradation half-life of 21.2 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).
Ground water:
Sediment:
Soil:
Biota: reported biological half-lives for pentachlorobiphenyls: $t_{½}$ = 155 to > 1000 d for trout, $t_{½}$ = 62–101 d for trout muscle; $t_{½}$ = 73 to > 200 d for carp (Niimi 1987)

7.1.1.124 2,3′,4′,5,5′-Pentachlorobiphenyl (PCB-124)



Common Name: 2,3′,4′,5,5′-Pentachlorobiphenyl
Synonym: PCB-124, 2′,3,4,5,5′-pentachloro-1,1′-biphenyl, 2′,3,4,5,5′-pentachlorobiphenyl
Chemical Name: 2,3′,4′,5,5′-pentachlorobiphenyl
CAS Registry No: 70424-70-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
  99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
  0.0336 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.00158 (20°C, supercooled liquid, Murphy et al. 1987)
  0.00326 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  1.01×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.00112 (GC-RI correlation, Burkhard et al. 1985b)
  2.60×10^{-4} (20°C, supercooled liquid P_L, Murphy et al. 1987)
  $\log (P_L/Pa) = -4688/(T/K) + 12.62$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  9.84 (calculated-P/C, Burkhard 1984)
  5.37 (20°C, calculated-P/C, Murphy et al. 1987)
  19.76 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
  5.70 (calculated-QSPR, Achman et al. 1993)
  17.65 (calculated-QSPR, Dunnivant et al. 1992)
  36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  6.36 (calculated-TSA, Burkhard 1984)
  6.73 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
  6.6178 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
  9.76 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.16	(suspended particulate matter, Burkhard 1984)
4.884	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

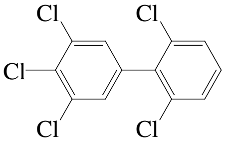
Ground water:

Sediment:

Soil:

Biota:

7.1.1.125 2,3′,4′,5′,6-Pentachlorobiphenyl (PCB-125)



Common Name: 2,3′,4′,5′,6-Pentachlorobiphenyl
Synonym: PCB-125
Chemical Name: 2,3′,4′,5′,6-pentachlorobiphenyl
CAS Registry No: 74472-39-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
73 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.87×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00204 (GC-RI correlation, Burkhard et al. 1985b)
0.0020 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4255/(T/K) + 12.45$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
14.5 (calculated-P/C, Burkhard 1984)
33.23 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
29.16 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)
6.51 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.2930 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.09	(suspended particulate matter, Burkhard 1984)
4.748	(marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

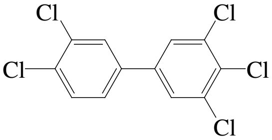
Ground water:

Sediment:

Soil:

Biota:

7.1.1.126 3,3′,4,4′,5-Pentachlorobiphenyl (PCB-126)



Common Name: 3,3′,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-126
Chemical Name: 3,3′,4,4′,5-pentachlorobiphenyl
CAS Registry No: 57465-28-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
106 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.158 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0321 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.000305 (generator column-GC/ECD, Hong & Qiao 1995)
0.00133* (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by van Noort 2004

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.736×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.05×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
4.86×10^{-4}, 2.86×10^{-4}(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.09×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4956/(T/K) + 13.31$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
2.51×10^{-4} (P_L, 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.776 (calculated-P/C, Burkhard et al. 1985)
5.471 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
8.39 (calculated-QSAR, Dunnivant et al. 1992)
21.02* ± 0.83 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 35.001 - 11847.5/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(98.5/\text{kJ·mol}^{-1})/RT] + (0.291/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
21.3 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 99 ± 9 kJ/mol, ΔS_H = 0.29 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.38 (calculated-TSA, Burkhard 1984)

6.57 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.89 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.6729 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.56; 6.62 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
7.00, 6.67 (calculated-MCI χ, calculated-MNDO-AMI method, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

10.61* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = –5.98 + 4870/(T/K); temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
11.77, 10.66; 10.61 (0, 20°C, GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.56 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.81, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor BSAF:

43 (trout, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:

6.18 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 5 (food lipid mg)/(g worm lipid-d); k_2 = 0.05 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.0137 d^{-1} with $t_{1/2}$ = 51 d (newly contaminated oysters, Gardinali et al. 2004)
k_2 = 0.0116 d^{-1} with $t_{1/2}$ = 60 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{1/2}$ = 304 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).

Ground water:

Sediment:

Soil:

Biota: reported biological half-lives for pentachlorobiphenyls: $t_{1/2}$ = 155 to > 1000 d for trout, $t_{1/2}$ = 62–101 d for trout muscle; $t_{1/2}$ = 73 to > 200 d for carp (Niimi 1987);

elimination $t_{1/2}$ = 13 d in earthworm given contaminated food (Wågman et al. 2001)

Depuration $t_{1/2}$ = 51 d for newly contaminated oysters, and $t_{1/2}$ = 60 d for chronically contaminated oysters (Gardinali et al. 2004)

TABLE 7.1.1.126.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 3,3′,4,4′,5-pentachlorobiphenyl (PCB 126) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
5	6.30×10^{-4}	4	0.958	–10	12.55
15	9.64×10^{-4}	11	2.82	0	11.81
25	1.33×10^{-3}	18	7.88	10	11.24
35	1.60×10^{-3}	25	21.02	20	10.61
		31	47.0	30	10.10
ln x = A –B/(T/K)					
	x	ln K_{AW} = –ΔH/RT + ΔS/R		ΔH_{OA}/(kJ mol^{-1}) = 93.25	
A		ΔS/R	35.012		
B	ΔH_{sol}/R	ΔH/R	11847.5	log K_{OA} = A + B/T	
				A	–5.979
mp/°C	160–161	enthalpy, entropy change:		B	4870
ΔH_{sol}/(kJ mol^{-1}) = 22.3		ΔH/(kJ·mol^{-1}) = 98.5 ± 9.4			
		ΔS/(J·mol^{-1}·K^{-1}) = 291 ± 32			

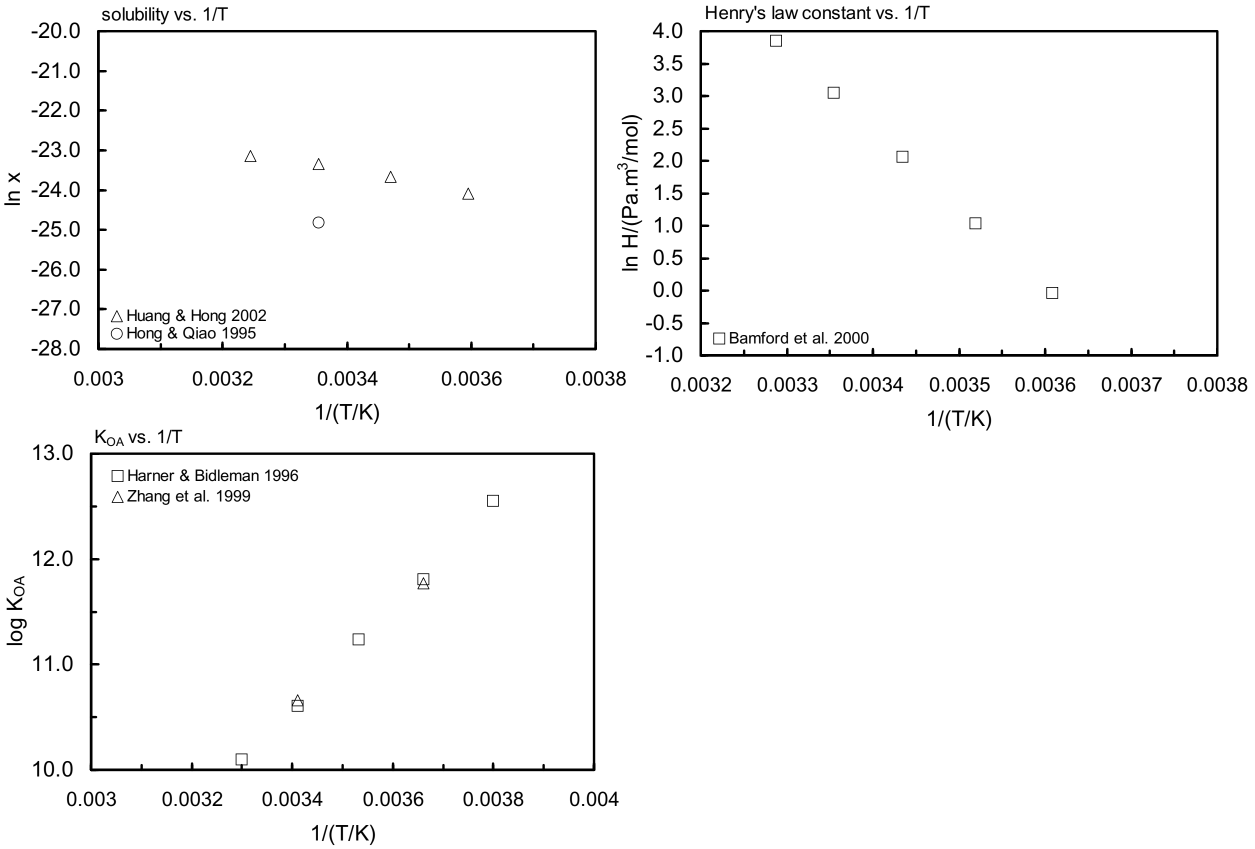
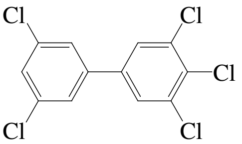


FIGURE 7.1.1.126.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 3,3′,4,4′,5-pentachlorobiphenyl (PCB-126).

7.1.1.127 3,3′,4,5,5′-Pentachlorobiphenyl (PCB-127)



Common Name: 3,3′,4,5,5′-Pentachlorobiphenyl
Synonym: PCB-127
Chemical Name: 3,3′,4,5,5′-pentachlorobiphenyl
CAS Registry No: 39635-33-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):

135	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

289.1	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0285	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.000651	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

4.04×10^{-4}	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000449	(GC-RI correlation, Burkhard et al. 1985b)
7.80×10^{-4}, 5.38×10^{-4}	(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

log (P_L/Pa) = –4956/(T/K) + 13.51 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

4.64	(calculated-P/C, Burkhard 1984)
34.45	(calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
12.73	(calculated-QSPR, Dunnivant et al. 1992)
21.3	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 99 ± 9 kJ/mol, ΔS_H = 0.29 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.42	(calculated-TSA, Burkhard 1984)
6.95	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.8023	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

10.53	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.22	(suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

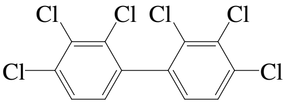
Ground water:

Sediment:

Soil:

Biota:

7.1.1.128 2,2′,3,3′,4,4′-Hexachlorobiphenyl (PCB-128)



Common Name: 2,2′,3,3′,4,4′-Hexachlorobiphenyl
Synonym: PCB-128, 2,2′,3,3′,4,4′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′-hexachlorobiphenyl
CAS Registry No: 38380-07-3
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
151 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3482
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.83 (Miller et al. 1984)
29.20 (Ruelle et al. 1993; Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
68.62 (Miller et al. 1984; Shiu & Mackay 1986)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0582 (Mackay et al. 1980; Shiu & Mackay 1 986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4.40×10^{-4} (generator column-GC/ECD, Weil et al. 1974)
9.90×10^{-4} (shake flask-GC/ECD, Dexter & Pavlou 1978)
2.85×10^{-4} (generator column-GC/ECD, Miller et al. 1984,1985)
0.0067 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
2.74×10^{-3}, 2.17×10^{-3}, 9.07×10^{-4}, 1.54×10^{-3} (RP-HPLC-k′ correlation, different stationary and mobile phase, Brodsky & Ballschmiter 1988)
0.0023 (generator column-GC, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.41×10^{-4} (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
3.59×10^{-4} (supercooled liquid P_L, Burkhard 1984)
2.31×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
3.59×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.67×10^{-4}, 2.94×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.83×10^{-5} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
3.67×10^{-4}, 2.94×10^{-4}, 3.41×10^{-4} (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
$\log (P/\text{mmHg}) = 11.40 - 5020/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
1.78×10^{-4}, 3.31×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4881/(T/K) + 12.91$ (GC-RT correlation, Falconer & Bidleman 1994)
$(2.90 - 154.0) \times 10^{-6}$; $(9.80 - 35.9) \times 10^{-5}$ (literature solid P_S range; supercooled liquid P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
50.66 (calculated, Murphy et al. 1983)
6.85 (calculated-P/C, Burkhard et al. 1985b)
11.91 (calculated-P/C, Shiu & Mackay 1986)

5.78 (20°C, calculated-P/C, Murphy et al. 1987)
3.04 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
50.5 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
1.32 (wetted-wall column-GC/ECD, Brunner et al. 1990)
10.51 (calculated-QSPR, Dunnivant et al. 1992)
0.890, 3.224, 10.99, 35.40 ± 1.5, 92.30 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 43.30 – 14193/(T/K); temp range 4–31°C (gas stripping-GC, Bamford 2000)
K_{AW} = exp[–(118.0/kJ·mol^{-1})/ RT] + (0.360/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
32.7 (exptl. data, Bamford et al. 2002)
ln K_{AW} = $-\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 118 ± 8 kJ/mol, ΔS_H = 0.36 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.44 (RP-TLC-RT correlation, Bruggeman et al. 1982)
6.98 (generator column-GC/ECD, Miller et al. 1984, 1985)
6.14 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.28 (HPLC-RP/MS correlation, Burkhard et al. 1985c)
6.50, 6.67, 6.83, 6.73 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.98 (generator column-GC/ECD, Doucette & Andren 1988)
7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
7.321 ± 0.027(shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
6.98, 6.87; 6.92, 6.87 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.71 (HPLC-k′ correlation, Neogrohati & Hammers 1992)
6.62 (generator column-GC, Larsen et al. 1992)
6.96 (recommended, Sangster 1993)
7.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.93 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
1.0 (poultry, Garten & Trabalka 1983)
4.28 (worms, Oliver 1987c)
5.77; 7.30 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
3.20–5.12 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.90–6.03 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.77, 7.31 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.41, 7.48 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
5.05 (calculated-MCI, Koch 1983)
6.42 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.06 (calculated-MCI, Bahnick & Doucette 1988)
5.26 (marine humic substance, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)
6.28, 6.17, 6.01 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
6.0 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.05 (soil, calculated-MCI, Sabljic et al. 1995)
5.93 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
6.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.00; 5.10 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Sorption Partition Coefficient, log K_{OM}:

5.05, 5.09 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Photooxidation: calculated room temp. rate constant for hexachlorobiphenyls is $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for gas-phase reaction with OH radicals, the tropospheric lifetime is calculated to be 29–60 d (Kwok et al. 1996).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 4970$ d^{-1}; $k_2 = 0.00843$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.009$ d^{-1} with $t_{1/2} = 75$ d and $k_2 = 0.012$ d^{-1} with $t_{1/2} = 59$ d for food concn of 8 ng/g and 99 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.005$ d^{-1} with $t_{1/2} = 146$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d^{-1} with $t_{1/2} = 205$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

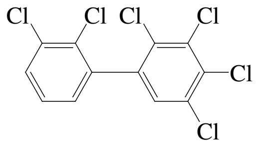
Soil:

Biota: $t_{1/2} > 1000$ d in rainbow trout, and $t_{1/2} = 89$ d in its muscle (Niimi & Oliver 1983).

Depuration $t_{1/2} = 59$–75 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 146$ d for high-dose treatment, $t_{1/2} = 205$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.129 2,2′,3,3′,4,5-Hexachlorobiphenyl (PCB-129)



Common Name: 2,2′,3,3′,4,5-Hexachlorobiphenyl
Synonym: PCB-129, 2,2′,3,3′,4,5-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5-hexachlorobiphenyl
CAS Registry No: 55215-18-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):

85	(Mackay et al. 1980; Bruggeman et al. 1982; Burkhard et al. 1985a; Opperhuizen et al. 1988; Brodsky & Ballschmiter 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3482
Molar Volume (cm^3/mol):

310.0	(calculated-Le Bas method at normal boiling point,)
237.4	(Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

0.256	(Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.00085	(generator column-GC/ECD, Weil et al. 1974)
0.0117	(20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00150, 0.00198, 0.000688, 0.00169	(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00582	(generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

5.76×10^{-4}	(GC-RI correlation, Burkhard et al. 1985a)
0.00208	(supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
4.68×10^{-4}	(supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)

$\log (P_L/Pa) = -4816/(T/K) + 12.80$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

39.52	(calculated-P/C, Burkhard et al. 1985b)
8.61	(calculated-MCI χ, Sabljic & Güsten 1989)
2.94	(wetted-wall column-GC, Brunner et al. 1990)
14.18	(calculated-QSPR, Dunnivant et al. 1992)
49.5	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.50	(HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.71, 6.71, 6.90. 6.71	(RP-HPLC-k′ correlations, Brodsky & Ballschmiter 1988)
6.94, 6.70; 6.81, 6.83	(multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.76 (recommended, Sangster 1993)
7.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.80 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
6.42 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.259 (marine humic substance, calculated-MCI χ, reported as association coefficient log K_h at 5 mg/L DOC, Sabljic 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.004$ d^{-1} with $t_{½} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

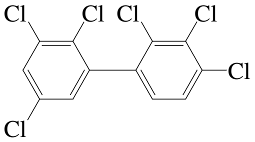
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½} = 156$ d for high-dose treatment, $t_{½} = 166$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.130 2,2′,3,3′,4,5′-Hexachlorobiphenyl (PCB-130)



Common Name: 2,2′,3,3′,4,5′-Hexachlorobiphenyl
Synonym: PCB-130, 2,2′,3,3′,4,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5′-hexachlorobiphenyl
CAS Registry No: 52663-66-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
96 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0168 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00569 (20°C, supercooled liquid, Murphy et al. 1987)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
5.35×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.92×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.61×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
4.17×10^{-4}, 5.75×10^{-4} (supercooled liquid P_L; GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4816/(T/K) + 12.89$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
11.55 (calculated-P/C, Burkhard 1984)
10.84 (20°C, calculated-P/C, Murphy et al. 1987)
19.45 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
3.75 (wetted wall column-GC/ECD, Brunner et al. 1990)
15.44 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 79 ± 18 kJ/mol, ΔS_H = 0.23 ± 0.06 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.57, 7.39 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapport & Eisenreich 1984)
6.98, 7.15; 6.79, 6.78 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.12 (recommended, Sangster 1993)
7.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.47	(suspended particulate matter, Burkhard 1984)
5.241	(marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004$ d^{-1} with $t_{1/2} = 184$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005$ d^{-1} with $t_{1/2} = 153$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

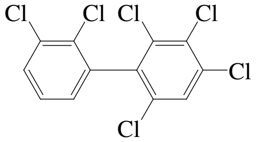
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 184$ d for high-dose treatment, $t_{1/2} = 153$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.131 2,2′,3,3′,4,6-Hexachlorobiphenyl (PCB-131)



Common Name: 2,2′,3,3′,4,6-Hexachlorobiphenyl
Synonym: PCB-131, 2,2′,3,3′,4,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,6-hexachlorobiphenyl
CAS Registry No: 61798-70-7
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
122 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0151 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01212 (20°C, supercooled liquid, Murphy et al. 1987)
0.00120 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.62×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00285 (GC-RI correlation, Burkhard et al. 1985b)
0.00126, 0.0107 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.63×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
6.92×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4681/(T/\text{K}) + 12.80$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
62.82 (calculated-P/C, Burkhard 1984)
6.59 (20°C, calculated-P/C, Murphy et al. 1987)
26.24 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
3.95 (wetted wall column-GC/ECD, Brunner et al. 1990; quoted, Achman et al. 1993)
24.53 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.78 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.97, 6.38; 6.41, 6.44 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.78 (recommended, Sangster 1993)
6.82 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

10.92, 9.83	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.05	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.51	(suspended particulate matter, Burkhard 1984)
5.100	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

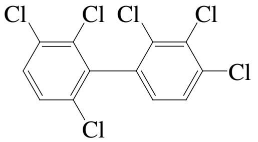
Ground water:

Sediment:

Soil:

Biota:

7.1.1.132 2,2′,3,3′,4,6′-Hexachlorobiphenyl (PCB-132)



Common Name: 2,2′,3,3′,4,6′-Hexachlorobiphenyl
Synonym: PCB-132, 2,2′,3,3′,4,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,6′-hexachlorobiphenyl
CAS Registry No: 38380-05-1
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
81 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0149 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00808 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00720 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.155×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.27×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
7.58×10^{-4}, 9.08×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.62×10^{-4}, 1.0×10^{-3} (supercooled liquid P_L: GC-RI correlations, different stationary phase, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4681/(T/\text{K}) + 12.5$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
27.97 (calculated-P/C, Burkhard 1984)
16.31 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
4.46 (wetted wall column-GC/ECD, Brunner et al. 1990)
2.42 (calculated-QSPR, Achman et al. 1993)
20.55 (calculated-QSPR, Dunnivant et al. 1992)
16.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
59.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 61 \pm 7$ kJ/mol, $\Delta S_H = 0.17 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.70 (HPLC-RT correlation, Shaw & Connell 1982)
6.20 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.09. 6.77; 6.63, 6.58 (multi-column-HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.20 (recommended, Sangster 1993)
7.04 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

11.16, 10.07; 9.96 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.76 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.52 (suspended particulate matter, Burkhard 1984)
5.10 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

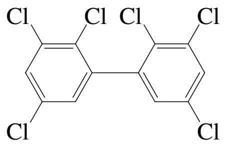
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16 – 0.5) × 10^{-12} cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.005 d^{-1} with $t_{½}$ = 136 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.005 d^{-1} with $t_{½}$ = 147 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 136 d for high-dose treatment, $t_{½}$ = 147 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.133 2,2′,3,3′,5,5′-Hexachlorobiphenyl (PCB-133)



Common Name: 2,2′,3,3′,5,5′-Hexachlorobiphenyl
Synonym: PCB-133, 2,2′,3,3′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,5′-hexachlorobiphenyl
CAS Registry No: 35694-04-3
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
129 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0954 (mp at 129°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0149 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
4.37×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.98×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
8.24×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
8.43×10^{-4}, 0.00110 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/\text{Pa}) = -4816/(T/\text{K}) + 13.08$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
19.25 (calculated-P/C, Burkhard 1984)
33.84 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.64 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.72 (calculated-TSA, Burkhard 1984)
6.86 (calculated-TSA, Hawker & Connell 1988a)
6.97, 7.02; 6.66, 6.60 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.63, 7.00 (quoted average values of GC-RV and HPLC-k′ correlations of Risby et al. 1990, Sangster 1993)
7.07 (recommended, Hansch et al. 1995)
6.7470 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
7.69 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.57	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.52	(suspended particulate matter, Burkhard 1984)
5.222	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

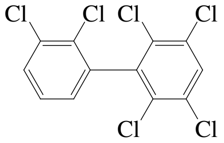
Ground water:

Sediment:

Soil:

Biota:

7.1.1.134 2,2′,3,3′,5,6-Hexachlorobiphenyl (PCB-134)



Common Name: 2,2′,3,3′,5,6-Hexachlorobiphenyl
Synonym: PCB-134, 2,2′,3,3′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,6-hexachlorobiphenyl
CAS Registry No: 52704-70-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
  100 (Mackay et al. 1980; Burkhard et al. 1985a; Kühne et al. 1995; Ruelle & Kesselring 1997)
  132 (Ran et al. 2002)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3482
Molar Volume (cm^3/mol):
  310.0 (calculated-Le Bas method at normal boiling point)
  237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.181 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.00091 (generator column-GC/ECD, Weil et al. 1973)
  0.0081 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  1.46×10^{-4} (calculated-S × HLC, Burkhard et al. 1985a)
  0.00246 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  4.83×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
  0.00127, 0.00185 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  3.60×10^{-4} (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  $\log (P/mmHg) = 11.30 - 4940/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
  7.41×10^{-4}, 1.32×10^{-3} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
  $\log (P_L/Pa) = -4681/(T/K) + 12.79$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
  57.76 (Murphy et al. 1983)
  55.53 (calculated-P/C, Burkhard et al. 1985b)
  9.83 (20°C, calculated-P/C, Murphy et al. 1987)
  20.67 (calculated-QSPR MCI χ, Sabljic & Güsten 1989)
  4.96 (wetted-wall column-GC/ECD, Brunner et al. 1990)
  32.27 (calculated-QSPR, Dunnivant et al. 1992)
  25.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  68.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 6$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.81 (generator column-GC/ECD,. Doucette & Andren 1987)
6.20 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.22, 6.43; 6.40, 6.44 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.20 (recommended, Sangster 1993)
6.91 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.80, 9.71 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.72 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.49 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.18, 5.16, 5.15, 4.41 (humic substances, in concentrations. of 5, 10, 20, 40 mg C/L, reported as log K_h, Lara & Ernst 1989)
5.18, 5.10 (marine humic substances, quoted, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)

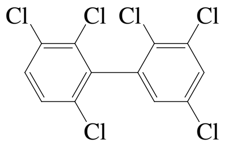
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, and Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

7.1.1.135 2,2′,3,3′,5,6′-Hexachlorobiphenyl (PCB-135)



Common Name: 2,2′,3,3′,5,6′-Hexachlorobiphenyl
Synonym: PCB-135, 2,2′,3,3′,5,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,6′-hexachlorobiphenyl
CAS Registry No: 52744-13-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
 102 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
 310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
 0.0133 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
 0.01294 (20°C, supercooled liquid, Murphy et al. 1987)
 0.00546 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 0.00361 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 1.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
 0.00188 (GC-RI correlation, Burkhard et al. 1985b)
 0.00115, 0.00184 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 5.07×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
 0.000741, 0.00132 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/Pa) = -4861/(T/K) + 12.76$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
 46.81 (calculated-P/C, Burkhard 1984)
 14.19 (20°C, calculated-P/C, Murphy et al. 1987)
 30.8 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
 5.67 (wetted wall column-GC/ECD, Brunner et al. 1990)
 27.21 (calculated-QSPR, Dunnivant et al. 1992)
 26.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
 69.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 45 \pm 3$ kJ/mol, $\Delta S_H = 0.12 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
 5.94, 7.15 (RP-HPLC-k′ correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
 6.32 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 6.97, 6.95; 6.41, 6.40 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.32 (recommended, Sangster 1993)
7.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.78, 9.69 (0, 20°C, multicolumn GC-k′ correlation, Zhang et al. 1999)
9.71 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

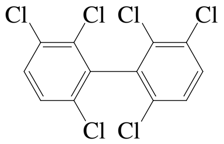
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.57 (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004$ d^{-1} with $t_{½} = 159$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½} = 192$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½} = 159$ d for high-dose treatment, $t_{½} = 192$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.136 2,2′,3,3′,6,6′-Hexachlorobiphenyl (PCB-136)



Common Name: 2,2′,3,3′,6,6′-Hexachlorobiphenyl
Synonym: PCB-136, 2,2′,3,3′,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,6,6′-hexachlorobiphenyl
CAS Registry No: 38411-22-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
112.05 (differential scanning calorimetry, Miller et al. 1984)
114.2 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.21 (differential scanning calorimetry, Miller et al. 1984)
21.10 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
54.81 (Miller et al. 1984)
Fugacity Ratio at 25°C, F:
0.138 (calculated, assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00099 (shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00603 (generator column-GC/ECD, Miller et al. 1984)
0.00451* (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
1.10×10^{-3}, 3.25×10^{-3}, 4.51×10^{-3}, 6.68×10^{-3} (4, 20, 25, 32°C, generator column-GC/ECD, Dickhut et al. 1986)
$\ln x = -5484.72/(T/K) - 3.8682$; temp range 4–32°C, ΔH_{ss} = 45.6 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
$\log x = -2378/(T/K) - 1.679$, ΔH_{ss} = 45.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
$S/(mol/L) = 2.39 \times 10^{-9} \exp(0.065 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
0.0202 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\ln x = -3.880235 - 5471.2/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.000531 (GC-RI correlation, Burkhard et al. 1985a)
0.00374 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00156, 0.00292 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00127 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00158, 0.00331 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4303/(T/K) + 11.63$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

93.22 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
22.79 (20°C, calculated-P/C, Murphy et al. 1987)
25.54 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
8.92 (wetted-wall column-GC/ECD, Brunner et al. 1990)
32.64 (calculated-QSPR, Dunnivant et al. 1992)
45.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
81.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

8.35 (Hansch & Leo 1979)
6.81 (generator column-HPLC, Woodburn et al. 1984)
6.63 (generator column-GC/ECD, Miller et al. 1984)
4.91 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.48 (HPLC-RP/MS correlation, Burkhard et al. 1985c)
6.81 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
5.76 (generator column-GC/ECD, Hawker & Connell 1988a)
7.118 ± 0.034(shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens)
7.18 (calculated-π const., De Bruijn et al. 1989)
6.63, 6.30; 6.30, 6.24 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.50 (calculated-UNIFAC activity coefficient, Dallos et al. 1993)
6.54 (recommended, Sangster 1993)
7.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.59, 9.53; 9.58 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.51 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

0.86 (poultry, Garten & Trabalka 1983)
5.43; 6.96 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.43, 6.96 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.53 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.53 (suspended solids, 0.7 mg/L, 43.2% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.68 (suspended solids, 6.5 mg/L, 14.8% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
4.95, 5.05, 4.95, 4.27 (marine humic substances in concentrations of 5, 10, 20, 40 mg L of DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
4.952, 4.942 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h. Observed; calculated-MCI χ, Sabljic et al. 1989)
6.01, 6.06, 5.90 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
6.04 (5.73–6.35) (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 18% at 24 h and 33% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 4390 d^{-1}; k_2 = 0.0181 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.005 d^{-1} with $t_{½}$ = 132 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 144 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{½}$ = 15.0 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

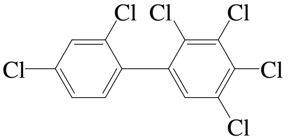
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 132 d for high-dose treatment, $t_{½}$ = 144 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.137 2,2′,3,4,4′,5-Hexachlorobiphenyl (PCB-137)



Common Name: 2,2′,3,4,4′,5-Hexachlorobiphenyl
Synonym: PCB-137, 2,2′,3,4,4′,5-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5-hexachlorobiphenyl
CAS Registry No: 35694-06-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
78.0 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.302 (mp at 78°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0158 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0084 (20°C, supercooled liquid, Murphy et al. 1987)
9.94×10^{-4}, 1.12×10^{-3}, 7.54×10^{-4}, 1.69×10^{-3} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.71×10^{-3} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.41×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.83×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.50×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
3.80×10^{-4}, 3.02×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phasess, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4816/(T/\text{K}) + 12.61$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
55.02 (calculated-P/C, Burkhard 1984)
6.89 (20°C, calculated-P/C, Murphy et al. 1987)
21.08 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
18.82 (calculated-QSPR, Dunnivant et al. 1992)
3.13 (calculated-QSPR, Achman et al. 1993)
13.0 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
55.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 69 \pm 8$ kJ/mol, $\Delta S_H = 0.20 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
> 6.89, > 7.71 (RP-HPLC-k′ correlation; uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
7.46 (HPLC-RT correlation, De Kock & Lord 1987)

6.84, 6.87, 6.88, 6.71 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.97, 7.06; 6.82, 6.78 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.83 (recommended, Sangster 1993)
7.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.89 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

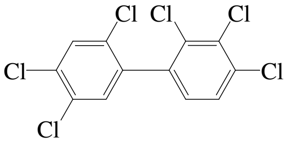
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.49 (suspended particulate matter, Burkhard 1984)
5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.94 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm³ molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004$ d^{-1} with $t_{½} = 186$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½} = 191$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½} = 186$ d for high-dose treatment, $t_{½} = 191$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.138 2,2′,3,4,4′,5′-Hexachlorobiphenyl (PCB-138)



Common Name: 2,2′,3,4,4′,5′-Hexachlorobiphenyl
Synonym: PCB-138, 2,2′,3,4,4′,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5′-hexachlorobiphenyl
CAS Registry No: 35065-28-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
79 (Hutzinger et al. 1974; Brodsky & Ballschmiter 1988)
80.5 (Kühne et al.1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)
247.4 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.286 (calculated, assuming ΔS_{fus} = 56 J/mol K, Mackay et al. 1992)
0.285 (calculated-ΔS_{fus} and mp, Passivirta et al. 1995)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0159 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.00729 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00173, 0.00158, 0.00122, 0.0015 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00181 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.0024 (calculated-MCI χ, Patil 1991)
0.00151 (calculated-QSPR, Dunnivant et al. 1992)
0.00268 (calculated-group contribution method, Kühne et al. 1995)
0.00268, 0.0072 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
$\log [S_L/(\text{mol/L})] = -1.12 + 1403/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
6.57×10^{-3} (calculated-mp and K_{OW}, Ran et al. 2002)
7.51×10^{-3}; 6.75×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)
$\log [S_L/(\text{mol m}^{-3})] = -1437/(T/K) + 0.093$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
5.06×10^{-4}, 5.65×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
1.58×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
4.87×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
5.10×10^{-4}, 4.96×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.33×10^{-4} (quoted average value from Bidleman 1984, Erickson 1986)
1.47×10^{-4} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 11.60 - 5040/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

3.31×10^{-4}, 4.90×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4800/(T/K) + 12.81$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
3.63×10^{-4} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
1.47×10^{-4}; 5.14×10^{-4} (solid, supercooled liquid, Passivirta et al. 1999)
$\log (P_S/Pa) = 15.76 - 5842/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 12.81 - 4800/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
5.37×10^{-4}; 5.62×10^{-4} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log (P_L/Pa) = -5034/(T/K) + 13.62$ (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
$\log (P_L/Pa) = -4770/(T/K) + 12.75$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

48.64	(calculated-P/C, Murphy et al. 1983)
11.04	(calculated-P/C, Burkhard et al. 1985b)
7.60	(20°C, calculated-P/C, Murphy et al. 1987)
10.84	(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.13	(wetted-wall column-GC, Brunner et al. 1990)
69.0	(Wittlinger & Ballschmiter 1990)
13.17	(calculated-QSPR, Dunnivant et al. 1992)

$\log [H/(Pa\ m^3/mol)] = 13.93 - 3757/(T/K)$ (Passivirta et al. 1999)
44.6* ± 1.7 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 31.152 - 10476.3/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(87.1/kJ\cdot mol^{-1})/RT + (0.259/kJ\cdot mol^{-1}\cdot K^{-1})/R]$; where $R = 8.314\ J\cdot K^{-1}\cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
45.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 87 \pm 7$ kJ/mol, $\Delta S_H = 0.26 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
39.81, 30.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -4672/(T/K) + 17.27$ (LDV linear regression of literature data, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -3332/(T/K) + 12.66$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.90 (HPLC-RT correlation, Shaw & Connell 1982)
6.62, 7.44 (RP-HPLC-RT correlation Rapaport & Eisenreich 1984)
6.67, 6.77, 6.73, 6.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.04, 6.80; 6.84, 6.79 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.42 (average, generator column-GC, Larsen et al. 1992)
6.92 (recommended, Sangster 1993)
7.25 (recommended, Hansch et al. 1995)
7.00, 7.22 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°Cor as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

10.09* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
$\log K_{OA} = -5.57 + 4584/(T/K)$; temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
9.51; 9.12 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
$\log K_{OA} = -5.17 + 4380/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
10.62 (10°C, estimated, Thomas et al. 1998)
11.34, 10.20; 10.18 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.09 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.76, 9.66 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

log K_{OA} = 4509/(T/K) – 5.37 (LDV linear regression of literature data, Li et al. 2003)
log K_{OA} = 4510/(T/K) – 5.47 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

5.88; 7.41 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
3.31–5.47 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.79–5.96 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.88, 7.42 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.42, 7.48 (mussel *Mytilus edilus*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 5.30 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.70 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.52–5.89 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

6.49 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.8–7.3, 6.6 (suspended sediment, average, Oliver 1987a)
7.60 (algae > 50 μm, Oliver 1987a)
6.65 (Lake Michigan water column, Swackhamer & Armstrong 1987)
5.21, 5.22, 5.17, 4.60 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.207, 5.241 (marine humic substances, quoted, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)
5.93 (soil from Ispra, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.50 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.04–7.28; 5.80–7.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.51; 6.28, 6.78, 6.41 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
6.27–7.44 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: photodegradation rate constant k = (0.08 ± 0.01) h^{-1} with $t_{½}$ = 8.2 h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16–0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.049 h^{-1}; k_2 = 0.008 h^{-1} (mayfly-sediment model II, Gobas et al. 1989)
k_1 = 4770 d^{-1}; k_2 = 0.00624 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.0344 d^{-1} with an elimination $t_{½}$ = 20.2 d (earthworm, Belfroid et al. 1995)
k_2 = 0.005 d^{-1} with $t_{½}$ = 139 d and k_2 = 0.011 d^{-1} with $t_{½}$ = 64 d for food concn of 31 ng/g and 176 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_1 = 0.00226 h^{-1}; k_2 = 0.145 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)

k_1(calc) = 5 (food lipid mg)/(g worm lipid-d); k_2(calc) = 0.05 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 186 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 191 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995);

$t_{½}$ = 6000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photodegradation $t_{½}$ = (8.2 ± 0.3) h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995);

$t_{½}$ = 120000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{½}$ = 19–25 yr (Geyer et al. 2000)

$t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{½}$ = of 20.d from earthworm (Belfroid et al. 1995)

Depuration $t_{½}$ = 64–139 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$t_{½}$ = 4.8 h in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination $t_{½}$ = 13 d in earthworm given contaminated food (predicted, Wågman et al. 2001)

depuration $t_{½}$ = 186 d for high-dose treatment, $t_{½}$ = 191 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.1.138.1
Reported Henry's law constants and octanol-air partition coefficients of 2,2′,3,4,4′,5′-hexachlorobiphenyl (PCB-138) at various temperatures and temperature dependence equations

Henry's law constant		log K_{OA}					
Bamford et al. 2000		Harner & Bidleman 1996		Kömp & McLachlan 1997		Zhang et al. 1999	
gas stripping-GC/MS		generator column-GC		fugacity meter-GC/MS		multicolumn-GC-k′ correlation	
t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}	t/°C	log K_{OA}	t/°C	log K_{OA}
4	2.88	–10	11.81	25	9.51	0	11.34
11	7.50	0	11.27			20	10.20
18	18.68	10	10.61				
25	44.6	20	10.09	log K_{OA} = A + B/T			
31	91.1	30	9.53	A	–5.17		
				B	4380		
		ΔH_{OA}/(kJ mol^{-1}) = 87.77		temp range 10–43°C			
enthalpy, entropy change:							
ΔH/(kJ·mol^{-1}) = 87.1 ± 7.4		log K_{OA} = A + B/T					
ΔS/(J·mol^{-1}·K^{-1}) = 259 ± 26		A	–5.568				
		B	4584				
ln K_{AW} = –ΔH/RT + ΔS/R							
eq. 1	K_{AW}						
A	31.1523						
B	10476						

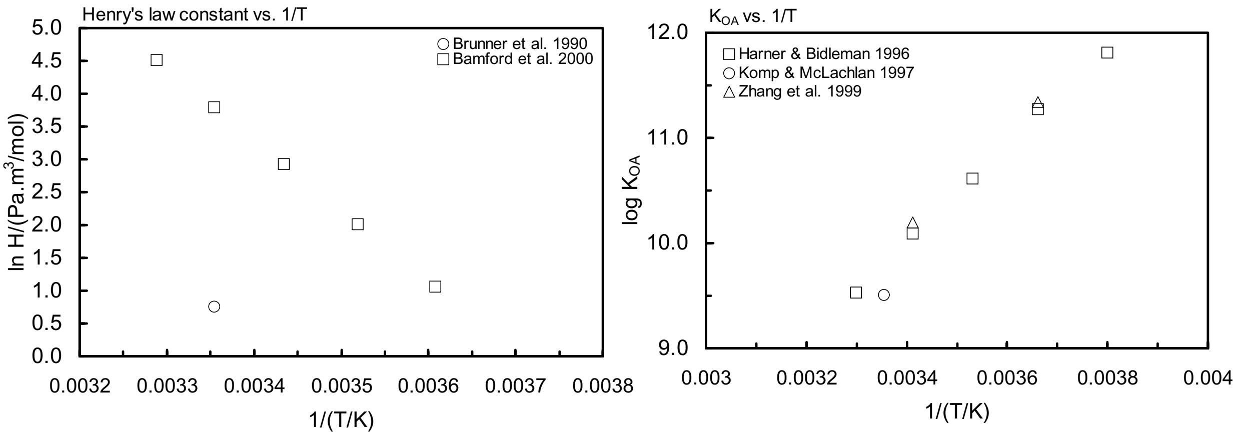
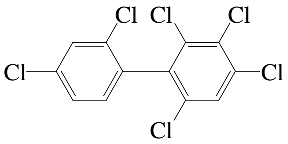


FIGURE 7.1.1.1.138.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,2′,3,4,4′,5′-hexachlorobiphenyl (PCB-138).

7.1.1.139 2,2′,3,4,4′,6-Hexachlorobiphenyl (PCB-139)



Common Name: 2,2′,3,4,4′,6-Hexachlorobiphenyl
Synonym: PCB-139
Chemical Name: 2,2′,3,4,4′,6-hexachlorobiphenyl
CAS Registry No: 56030-56-9
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
123 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0126 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.05×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.65×10^{-3}, 3.30×10^{-3}, 2.33×10^{-4} (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.26×10^{-3} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4681/(T/K) + 12.78$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
87.24 (calculated-P/C, Burkhard 1984)
38.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
33.32 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.79 (calculated-TSA, Burkhard 1984)
6.67 (calculated-TSA, Hawker & Connell 1988a)
7.12, 6.68; 6.54, 6.50 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.70 (recommended, Sangster 1993)
6.95 (recommended, Hansch et al. 1995)
6.6419 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.59	(suspended particulate matter, Burkhard 1984)
5.083	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

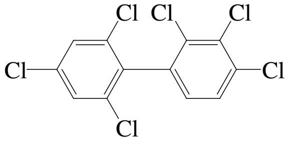
Ground water:

Sediment:

Soil:

Biota:

7.1.1.140 2,2′,3,4,4′,6′-Hexachlorobiphenyl (PCB-140)



Common Name: 2,2′,3,4,4′,6′-Hexachlorobiphenyl
Synonym: PCB-140, 2,2′,3,4,4′,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,6′-hexachlorobiphenyl
CAS Registry No: 59291-64-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
123 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0125 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00314, 0.00203, 0.0015, 0.00194 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00325 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
1.26×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00138 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
36.38 (calculated-P/C, Burkhard 1984)
43.06 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
31.17 (calculated-QSAR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.79 (calculated-TSA, Burkhard 1984)
6.48, 6.70, 6.47, 6.66 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.67 (calculated-TSA, Hawker & Connell 1988a)
7.01, 6.86; 6.56, 6.51 (multicolumn HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.58 (recommended, Sangster 1993).
6.97 (recommended, Hansch et al. 1995)
6.4851 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.59	(suspended particulate matter, Burkhard 1984)
5.083	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calc-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

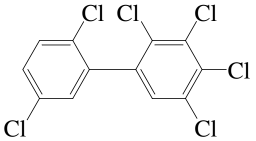
Ground water:

Sediment:

Soil:

Biota:

7.1.1.141 2,2′,3,4,5,5′-Hexachlorobiphenyl (PCB-141)



Common Name: 2,2′,3,4,5,5′-Hexachlorobiphenyl
Synonym: PCB-141, 2,2′,3,4,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,5′-hexachlorobiphenyl
CAS Registry No: 52712-04-6
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
85 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.258 (mp at 85°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0160 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00755 (20°C, supercooled liquid, Murphy et al. 1987)
0.00109, 0.00150, 0.00134, 0.00165 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0025 (calculated-group contribution method, Kühne et al. 1995)
0.00244, 0.00642 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00295 (GC-RI correlation, Burkhard et al. 1985b)
2.05×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 11.50 - 5080/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
5.01×10^{-4}, 6.46×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4816/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
61.5 (calculated-P/C, Burkhard 1984)
9.83 (20°C,calculated-P/C, Murphy et al. 1987)
14.49 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
2.33 (wetted wall column-GC/ECD, Brunner et al. 1990)
17.61 (calculated-QSPR, Dunnivant et al. 1992)
6.54 (calculated-QSPR, Achman et al. 1993)
12.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
54.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 70 \pm 7$ kJ/mol, $\Delta S_H = 0.20 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.69 (calculated-TSA, Burkhard 1984)
6.80, 6.79, 6.79, 6.71 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.82 (calculated-TSA, Hawker & Connell 1988a)
6.98, 7.02; 6.78, 6.73 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.75 (recommended, Sangster 1993)
9.538 (calculated-UNIFAC group contribution, Chen et al. 1993)
7.19 (recommended, Hansch et al. 1995)
7.10, 6.64–6.89 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
6.70 (estimated, Girvin & Scott 1997)
6.8226 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.55 (10°C, estimated, Thomas et al. 1998)
11.18, 10.07; 10.13 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.87 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.81; 7.34 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

6.49 (suspended particulate matter, Burkhard 1984)
5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.05 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.20 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)
6.02 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 4910\ d^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.00764\ d^{-1}$ (22°C, zebrafish, 30-d clearance, Fox et al. 1994)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 171$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 198$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

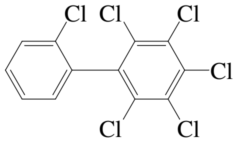
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 171 d for high-dose treatment, $t_{1/2}$ = 198 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.142 2,2′,3,4,5,6-Hexachlorobiphenyl (PCB-142)



Common Name: 2,2′,3,4,5,6-Hexachlorobiphenyl
Synonym: PCB-142, 2,2′,3,4,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,6-hexachlorobiphenyl
CAS Registry No: 41411-61-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):

136.0	(Burkhard et al. 1985b)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

310.0	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0815 (mp at 136°C)

Water Solubility (g/m^3 or mg/L at 25°C):

0.0171	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00361	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00138	(calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):

3.41×10^{-3}	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000293	(GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):

71.74	(calculated-P/C, Burkhard 1984)
21.18	(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
31.89	(calculated-QSPR, Dunnivant et al. 1992)
68.8	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

6.66	(calculated-TSA, Burkhard 1984)
6.51	(calculated-TSA, Hawker & Connell 1988)
6.94, 6.75; 6.56, 6.41	(multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.85	(recommended, Sangster 1993)
6.97	(recommended, Hansch et al. 1995)
6.5729	(calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.84	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.46	(suspended particulate matter, Burkhard 1984)
5.119	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16–0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

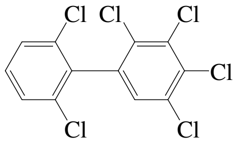
Ground water:

Sediment:

Soil:

Biota:

7.1.1.143 2,2′,3,4,5,6′-Hexachlorobiphenyl (PCB-143)



Common Name: 2,2′,3,4,5,6′-Hexachlorobiphenyl
Synonym: PCB-143, 2,2′,3,4,5,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,6′-hexachlorobiphenyl
CAS Registry No: 68194-15-0
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
116 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0143 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00287, 0.00238, 0.00250, 0.00293 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.046×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.41×10^{-3} (P_L supercooled liquid values: GC-RI correlation, Burkhard et al. 1985b)
9.014×10^{-4}, 9.59×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
7.41×10^{-4}, 1.35×10^{-3} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4681/(T/\text{K}) + 12.65$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
127.7 (calculated-P/C, Burkhard 1984)
25.94 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
3.95 (wetted wall column-GC/ECD, Brunner et al. 1990)
29.83 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 9$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.74 (calculated-TSA, Burkhard 1984)
6.52, 6.65, 6.51, 6.55 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.60 (calculated-TSA, Hawker & Connell 1988)
6.89, 6.63; 6.51, 6.48 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.56	(recommended, Sangster 1993)
6.92	(recommended, Hansch et al. 1995)
6.545	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.64	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.54	(suspended particulate matter, Burkhard 1984)
5.100	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 3 (food lipid mg)/(g worm lipid-d); k_2 = 0.07 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

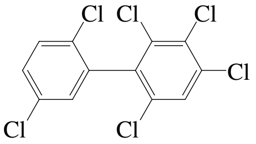
Ground water:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 10 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.144 2,2′,3,4,5′,6-Hexachlorobiphenyl (PCB-144)



Common Name: 2,2′,3,4,5′,6-Hexachlorobiphenyl
Synonym: PCB-144, 2,2′,3,4,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5′,6-hexachlorobiphenyl
CAS Registry No: 68194-14-9
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
110 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0126 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01294 (20°C, supercooled liquid, Murphy et al. 1987)
0.00353 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.45×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00371 (GC-RI correlation, Burkhard et al. 1985b)
5.07×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
0.00166, 0.00105 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4681/(T/\text{K}) + 12.70$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
98.23 (calculated-P/C, Burkhard 1984)
14.19 (20°C, calculated-P/C, Murphy et al. 1987)
32.22 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
5.70 (calculated-QSPR, Achman et al. 1993)
29.97 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.79 (calculated-TSA, Burkhard 1984)
6.45 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.67 (calculated-TSA, Hawker & Connell 1988a, 1990)
6.96, 6.68; 6.38, 6.29 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.45 (recommended, Sangster 1993)
6.79 (recommended, Hansch et al. 1995)

6.70	(estimated, Girvin & Scott 1997)
6.6482	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.73, 9.62; 9.62 (0, 20°C, multi-column GC-k′ correlation; calc at 20°C, Zhang et al. 1999)

10.15	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.59	(suspended particulate matter, Burkhard 1984)
5.083	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.20	(soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005\ d^{-1}$ with $t_{½} = 137$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 184$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

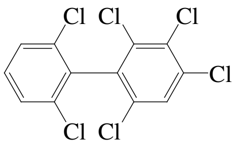
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 137 d for high-dose treatment, $t_{½}$ = 184 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.145 2,2′,3,4,6,6′-Hexachlorobiphenyl (PCB-145)



Common Name: 2,2′,3,4,6,6′-Hexachlorobiphenyl
Synonym: PCB-145, 2,2′,3,4,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,6,6′-hexachlorobiphenyl
CAS Registry No: 74472-40-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):

84	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

310.0	(calculated-Le Bas method)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0137	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0181	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

6.36×10^{-3}	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00681	(GC-RI correlation, Burkhard et al. 1985b)
0.00309	(supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)

log (P_L/Pa) = –4303/T + 11.90 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

168.2	(calculated-P/C, Burkhard 1984)
41.34	(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
46.61	(calculated-QSPR, Dunnivant et al. 1992)
81.5	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 27 ± 5 kJ/mol, ΔS_H = 0.06 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.76	(calculated-TSA, Burkhard 1984)
6.25	(calculated-TSA, Hawker & Connell 1988a)
6.92, 6.59; 6.30, 6.26	(multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phase, Risby et al. 1990)
6.28, 6.78	(quoted average values of Risby et al. 1990, Sangster 1993)
6.71	(recommended, Hansch et al. 1995)
6.2606	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.94	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.56	(suspended particulate matter, Burkhard 1984)
4.942	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.16 – 0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

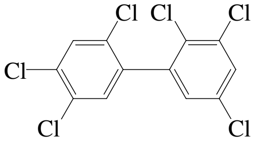
Ground water:

Sediment:

Soil:

Biota:

7.1.1.146 2,2′,3,4′,5,5′-Hexachlorobiphenyl (PCB-146)



Common Name: 2,2′,3,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-146, 2,2′,3,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 51908-16-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
90 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00759 (20°C, supercooled liquid, Murphy et al. 1987)
0.00095 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.28×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000801 (GC-RI correlation, Burkhard et al. 1985b)
7.73×10^{-4}, 9.614×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.87×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
6.31×10^{-4}, 8.51×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4816/(T/\text{K}) + 13.04$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
18.54 (calculated-P/C, Burkhard 1984)
8.92 (20°C, calculated-P/C, Murphy et al. 1987)
25.23 (calculated-QSAR- MCI χ, Sabljic & Güsten 1989)
2.53 (wetted wall column-GC/ECD, Brunner et al. 1990; quoted, Achman et al. 1993)
19.0 (calculated-QSPR, Dunnivant et al. 1992)
17.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
60.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 59 \pm 7$ kJ/mol, $\Delta S_H = 0.17 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.74 (calculated-TSA, Burkhard 1984)
6.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.89 (calculated-TSA, Hawker & Connell 1988a)

7.02, 7.08; 6.71, 6.71 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.57 (generator column-GC, Larsen et al. 1992)
6.85 (recommended, Sangster 1993)
7.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.96, 9.84 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.97 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

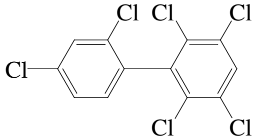
Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.80, 5.30 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:
6.54 (suspended particulate matter, Burkhard 1984)
5.40 (Lake Superior suspended solids, GC/ECD, Baker et al. 1986)
5.18, 5.22, 5.14, 4.58 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.18; 5.22 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
5.87 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.20 (colloids and micro-particulates from precipitation events, Murray & Andren 1992)
6.20 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)
6.01 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16 – 0.5) × 10^{-12} cm³ molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.004 d^{-1} with $t_{½}$ = 166 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{½}$ = 216 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 166 d for high-dose treatment, $t_{½}$ = 216 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.147 2,2′,3,4′,5,6-Hexachlorobiphenyl (PCB-147)



Common Name: 2,2′,3,4′,5,6-Hexachlorobiphenyl
Synonym: PCB-147, 2,2′,3,4′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,6-hexachlorobiphenyl
CAS Registry No: 68194-13-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):

116	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

310.0	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0134	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00287	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

2.86×10^{-3}	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00309	(GC-RI correlation, Burkhard et al. 1985b)

log (P/mmHg) = 11.20 – 4910/(T/K) (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant (Pa·m^3/mol at 25°C):

77.21	(calculated-P/C, Burkhard 1984)
32.63	(calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
5.17	(wetted wall column-GC/ECD, Brunner et al. 1990)
31.97	(calculated-QSPR, Dunnivant et al. 1992)
5.70	(calculated-QSPR, Achman et al. 1993)
68.8	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.77	(calculated-TSA, Burkhard 1984)
6.64	(calculated-TSA, Hawker & Connell 1988a)
7.07, 6.73, 6.52, 6.51	(multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.52, 6.90	(quoted average values of Risby et al. 1990, Sangster 1993)
6.93	(recommended, Hansch et al. 1995)
6.6069	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.79, 9.672	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.70	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.57 (suspended particulate matter, Burkhard 1984)

5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.16 – 0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{½}$ = 194 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.002 d^{-1} with $t_{½}$ = 283 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

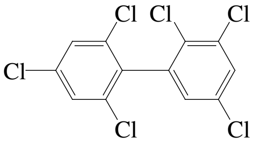
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 194 d for high-dose treatment, $t_{½}$ = 283 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.148 2,2′,3,4′,5,6′-Hexachlorobiphenyl (PCB-148)



Common Name: 2,2′,3,4′,5,6′-Hexachlorobiphenyl
Synonym: PCB-148, 2,2′,3,4′,5,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,6′-hexachlorobiphenyl
CAS Registry No: 74472-42-7
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
104 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0112 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0369 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.87×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00204 (GC-RI correlation, Burkhard et al. 1985b)
0.00190, 0.00277 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/\text{Pa}) = -4681/(T/K) + 12.98$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
60.69 (calculated-P/C, Burkhard 1984)
57.65 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
43.52 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.84 (calculated-TSA, Burkhard 1984)
5.74 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.73 (calculated-TSA, Hawker & Connell 1988a)
7.04, 6.74; 6.46, 6.44 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
5.74 (recommended, Sangster 1993)
6.87 (recommended, Hansch et al. 1995)
6.6291 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.51	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.64	(suspended particulate matter, Burkhard 1984)
5.064	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
5.707	(Ispra soil, shake flask-GC, Paya-Perez et al. 1991)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

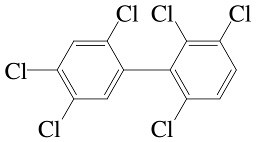
Ground water:

Sediment:

Soil:

Biota:

7.1.1.149 2,2′,3,4′,5′,6-Hexachlorobiphenyl (PCB-149)



Common Name: 2,2′,3,4′,5′,6-Hexachlorobiphenyl
Synonym: PCB-149, 2,2′,3,4′,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5′,6-hexachlorobiphenyl
CAS Registry No: 38380-04-0
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 369.9
Melting Point (°C):
oil (Erickson 1986)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0127 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01217 (20°C, supercooled liquid, Murphy et al. 1987)
0.00414 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00454 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.124×10^{-3}, 1.83×10^{-3} (P_L supercooled liquid, GC-RT correlation, different stationary phases, Bidleman 1984)
1.57×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.72×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
0.00105, 0.00158 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.47×10^{-3} (P_L supercooled liquid, quoted average value of Bidleman 1984, Erickson 1986)
4.96×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
8.51×10^{-4}, 1.48×10^{-3} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4689/(T/K) + 12.78$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
44.79 (calculated-P/C, Burkhard 1984)
15.0 (20°C, calculated-P/C, Murphy et al. 1987)
22.09 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
4.32 (calculated-QSPR, Achman et al. 1993)
24.03 (calculated-QSPR, Dunnivant et al. 1992)
0.682; 1.994 (0, 15°C, Hornbuckle et al. 1994)
25.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
68.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 7$ kJ/mol, $\Delta S_H = 0.12 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.70 (HPLC-RT correlation, Shaw & Connell 1982)
6.14, 7.28 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

6.79 (calculated-TSA, Burkhard 1984)
6.41 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.67 (calculated-TSA, Hawker & Connell 1988a)
7.02, 7.0; 6.45, 6.47 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.54 (generator column-GC, Larsen et al. 1992)
6.41 (recommended, Sangster 1993)
6.86 (recommended, Hansch et al. 1995)
6.4731 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
9.27; 8.68 (generator column; calculated-K_{OW}/K_{AW}, Kömp & McLachlan 1997a)
$\log K_{OA} = -6.50 + 4700/(T/K)$, temp range 10–43°C (Kömp & McLachlan 1997a)
9.27 (quoted, Kömp & McLachlan 1997b)
10.83, 9.74; 9.80 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.78 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

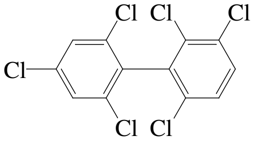
Biota Sediment Accumulation Factor, BSAF:
105 (trout, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:
6.59 (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
5.79 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.10 (colloids and micro-particulates from precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc)$ = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 = 0.00097$ h^{-1}; $k_2 = 0.240$ h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
$k_2 = 0.004$ d^{-1} with $t_{1/2}$ = 162 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003$ d^{-1} with $t_{1/2}$ = 199 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{1/2}$ = 162 d for high-dose treatment, $t_{1/2}$ = 199 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.150 2,2′,3,4′,6,6′-Hexachlorobiphenyl (PCB-150)



Common Name: 2,2′,3,4′,6,6′-Hexachlorobiphenyl
Synonym: PCB-150, 2,2′,3,4′,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,6,6′-hexachlorobiphenyl
CAS Registry No: 68194-08-1
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
104 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0121 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00907 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
4.07×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00438 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
121.6 (calculated-P/C, Burkhard 1984)
52.18 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
51.25 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.81 (calculated-TSA, Burkhard 1984)
6.32 (calculated-TSA, Hawker & Connell 1988a)
6.69; 6.59; 6.34, 6.27 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.64, 6.31 (quoted average values of Risby et al. 1990, Sangster 1993)
6.75 (recommended, Hansch et al. 1995)
6.1643 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.61	(suspended particulate matter, Burkhard 1984)
4.924	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

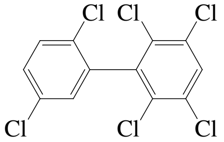
Ground water:

Sediment:

Soil:

Biota:

7.1.1.151 2,2′,3,5,5′,6-Hexachlorobiphenyl (PCB-151)



Common Name: 2,2′,3,5,5′,6-Hexachlorobiphenyl
Synonym: PCB-151, 2,2′,3,5,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5,5′,6-hexachlorobiphenyl
CAS Registry No: 52663-63-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
101 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.180 (mp at 101°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0134 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01355 (20°C, supercooled liquid, Murphy et al. 1987)
0.00454, 0.00414, 0.00487, 0.00337 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00720 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00223 (calculated-QSPR, Dunnivant et al. 1992)
0.00203 (calculated-group contribution method, Kühne et al. 1995)
0.00173, 0.00454 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.00559 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.32×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.16×10^{-3}, 1.67×10^{-4}, 2.23×10^{-4} (calculated-MW, GC-RI correlation, MCI χ, Burkhard et al. 1985b)
0.00177, 0.00255 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.97×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 11.30 - 4910/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
1.91×10^{-3} (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4681/(T/K) + 12.95$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
86.94 (calculated-P/C, Burkhard 1984)
15.91 (20°C, calculated-P/C, Murphy et al. 1987)
52.18 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
5.98 (wetted wall column-GC/ECD, Brunner et al. 1990)
28.69 (calculated-QSPR, Dunnivant et al. 1992)
33.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)

73.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 37 \pm 5$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
6.38, 6.49, 6.32, 6.51 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.64 (calculated-TSA, Hawker & Connell 1988a)
6.95, 7.35; 6.44, 6.43 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.45 (generator column-GC, Larsen et al. 1992)
6.43 (recommended, Sangster 1993)
6.85 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.08 (10°C, estimated, Thomas et al. 1998)
10.68, 9.58 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.68 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:
5.54; 7.07 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:
6.56 (suspended particulate matter, Burkhard 1984)
5.03, 5.11, 5.09, 4.41 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.031; 5.083 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
6.05, 6.05, 5.93 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.79 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
4.99, 4.82; 4.85 (sediments from Brown's Lake, Helmet City Lake; WES reference soil, shake flask-HPLC/fluorescence, Brannon et al. 1995)
6.20 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)
5.75 (4.96–6.18) (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 = 4220$ d^{-1}; $k_2 = 0.0121$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.004$ d^{-1} with $t_{1/2} = 174$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{1/2} = 196$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

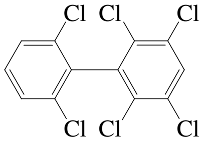
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 174 d for high-dose treatment, $t_{1/2}$ = 196 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.152 2,2′,3,5,6,6′-Hexachlorobiphenyl (PCB-152)



Common Name: 2,2′,3,5,6,6′-Hexachlorobiphenyl
Synonym: PCB-152, 2,2′,3,5,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5,6,6′-hexachlorobiphenyl
CAS Registry No: 68914-09-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):

111	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

310.0	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0145	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0114	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):

5.95×10^{-3}	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00638	(GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):

147.9	(calculated-P/C, Burkhard 1984)
35.57	(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
43.32	(calculated-QSPR, Dunnivant et al. 1992)
81.5	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 27 ± 5 kJ/mol, ΔS_H = 0.06 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.73	(calculated-TSA, Burkhard 1984)
6.22	(calculated-TSA, Hawker & Connell 1988a;)
6.86, 6.36; 6.10, 6.09	(multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.61, 6.10	(average values of Risby et al. 1990, Sangster 1993)
6.51	(recommended, Hansch et al. 1995)
6.2295	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.44	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.53	(suspended particulate matter, Burkhard 1984)
4.942	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16–0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

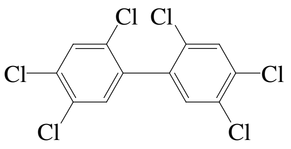
Ground water:

Sediment:

Soil:

Biota:

7.1.1.153 2,2′,4,4′,5,5′-Hexachlorobiphenyl (PCB-153)



Common Name: 2,2′,4,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-153, 2,2′,4,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 35065-27-1
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
103.5 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999; Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.90 (Opperhuizen et al. 1987; Ruelle et al. 1993)
17.50 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.169 (calculated, assuming ΔS_{fus} = 56 J/mol K, Mackay et al. 1980; Shiu & Mackay 1986)
0.167 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0088 (shake flask-GC/ECD, Wallnöfer et al. 1973)
0.0012 (generator column-GC/ECD, Weil et al. 1974)
9.53×10^{-4} (shake flask-GC/ECD, Haque & Schmedding 1975)
9.50×10^{-4} (24°C, shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977)
0.00105 (16.5°C, shake flask-GC/ECD, Wiese & Griffin 1978)
6.9×10^{-5} (calculated-UNIFAC activity coefficients, Banerjee 1985)
0.00914 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
8.86×10^{-4}, 9.4×10^{-4}, 1.34×10^{-3}, 1.5×10^{-3} (RP-HPLC-k′correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.28×10^{-5} (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.60×10^{-4} (generator column-GC/ECD, Dunnivant & Elzerman 1988)
8.45×10^{-3}* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988)
4.62×10^{-3}, 8.45×10^{-3}, 1.28×10^{-2} (4, 25, 40°C, generator column-GC/ECD, Doucette & Andren 1988)
$S/(mol/L) = 1.15 \times 10^{-8} \exp(0.028 \cdot t/°C)$ (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
$\log x = -1059/(T/K) - 5.819$, temp range 4–40°C, ΔH_{ss} = 20.3 kJ/mol (generator column-GC/ECD, Doucette & Andren 1988a)
0.00115 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
$\log [S_L/(mol/L)] = -1.20 - 1113/(T/K)$ (supercooled liquid S_L, Passivirta et al. 1999)
$\ln x = -13.37313 - 2445.3/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0136, 0.0111 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log [S_L/(mol\ m^{-3})] = -1305/(T/K) + 0.14$ (supercooled liquid S_L, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6.80×10^{-4}, 7.19×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
6.63×10^{-3} (supercooled liquid P_L, GC-RT correlation Burkhard 1984)
1.24×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
6.63×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
7.08×10^{-4}, 8.13×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.57×10^{-4} (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985b)
1.19×10^{-4}; 7.0×10^{-4} (selected values: solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
2.53×10^{-4} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 11.40 - 5040/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
7.0×10^{-4} (supercooled liquid P_L, Dunnivant & Elzerman 1988)
5.60×10^{-4} (Wittlinger & Ballschmiter 1990)
5.62×10^{-4}, 7.24×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4775/(T/K) + 12.85$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
3.63×10^{-4} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
1.39×10^{-4}; 8.34×10^{-4} (solid; supercooled liquid, Passivirta et al. 1999)
$\log (P_S/\text{Pa}) = 15.80 - 5887/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 12.85 - 4775/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
$(3.20 - 124.0) \times 10^{-5}$; $(1.80 - 66.3) \times 10^{-4}$ (literature P_S range; literature P_L range, Delle Site 1997)
7.75×10^{-5} (estimated-EPIWIN v3.04, Hardy 2002)
5.25×10^{-4}; 6.03×10^{-4} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/\text{Pa} = -4923/(T/K) + 13.24$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log P_L/\text{Pa} = -4712/(T/K) + 12.59$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):
35.46 (calculated, Murphy et al. 1983)
12.46 (gas stripping-GC, Coates 1984)
17.93 (calculated-P/C, Burkhard et al. 1985b)
6.08 (20°C, batch stripping-GC, Oliver 1985)
42.9 (calculated-P/C, Shiu & Mackay 1986)
10.03 (20°C, calculated-P/C, Murphy et al. 1987)
13.37 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
50.34 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
2.33 (wetted-wall column-GC/ECD, Brunner et al. 1990)
16.70 (calculated-QSPR, Dunnivant et al. 1992)
13.98 ± 1.5, 13.48 ± 1.2 (gas stripping-GC/ECD, purge vessel's height at 26-cm; 67-cm; Girvin et al. 1997)
$\log [H/(\text{Pa m}^3/\text{mol})] = 14.05 - 3662/(T/K)$ (Passivirta et al. 1999)
52.8* ± 1.6 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 22.853 - 7950.45/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp\{-[66.1/(\text{kJ mol}^{-1})]/ RT\} + [0.190/(\text{kJ mol}^{-1}\ K^{-1})/R]$; where $R = 8.314\ J\ K^{-1}\ mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
54.0 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 66 \pm 5$ kJ/mol, $\Delta S_H = 0.19 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
6.94 (estimated-bond method EPIWIN v.3.04, Hardy 2002)
25.12, 19.95 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log H/(\text{Pa m}^3/\text{mol}) = -2584/(T/K) + 10.07$ (LDV linear regression of literature data, Li et al. 2003)
$\log H/(\text{Pa m}^3/\text{mol}) = -3407/(T/K) + 12.72$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
6.72 (shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977; Chiou et al. 1982)
8.35 (Hansch & Leo 1979)

6.34 (shake flask-GC/ECD, Karickhoff et al. 1979)
7.44 (RP-TLC-k′ correlation, Bruggeman et al. 1982; 1984)
6.93, 7.75 (RP-HPLC-RT correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.90 (generator column-HPLC, Woodburn et al. 1984)
6.68 (HPLC/MS correlation, Burkhard et al. 1985c)
7.69, 7.71 (HPLC-k′ correlation, calculated, De Kock & Lord 1987)
6.90 (generator column-GC/ECD, Doucette & Andren 1987,1988)
7.69 (HPLC-RT correlation, De Kock & Lord 1987)
7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.84, 6.90, 6.71, 6.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.82, 6.85 (RP-HPLC-k′ correlation, different stationary phases, Sherbolm & Eganhouse 1988)
7.00 (RP-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
7.07, 7.12; 6.75, 6.72 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.81 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.51 (average, generator column-GC, Larsen et al. 1992)
6.80 (recommended, Sangster 1993)
7.50 (recommended, Hansch et al. 1995)
6.58 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)
6.71, 6.87 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.50 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
10.04* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log $K_{OA} = -6.02 + 4696/(T/K)$; temp range –10 to +30°C (generator column-GC, Harner & Bidleman 1996)
9.37; 9.09 (fugacity meter/generator column-GC; measured range 10–43°C, calculated, Kömp & McLachlan 1997a)
log $K_{OA} = -5.49 + 4430/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
10.50 (10°C, estimated, Thomas et al. 1998)
11.03, 9.99; 10.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.80; 9.65 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
9.52, 9.44 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log $K_{OA} = 4966/(T/K) - 7.14$ (LDV linear regression of literature data, Li et al. 2003)
log $K_{OA} = 3785/(T/K) - 7.00$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:

4.68 (oyster, Vreeland 1974)
4.66 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
4.48, 5.23 (calculated-S, K_{OC}, Kenaga 1980)
5.23, 3.76 (amphipods, clams, Lynch et al. 1982)
5.03, 4.88, 4.65 (algae, snail, aquatic earthworm, Lynch et al. 1982)
4.82, 4.63 (crayfish, fish, Lynch et at. 1982)
4.00, 4.72, 3.77 (calculated-S, calculated-C, calculated-K_{OW}, Lynch et al. 1982)
0.99 (poultry, Garten & Trabalka 1983)
6.78 (guppy, 3.5% lipid, Bruggeman et al. 1982, 1984)
4.84 (rainbow trout, ratio of uptake and depuration rate constants, Muir et al. 1985)
5.87; 6.00 (rainbow trout: laboratory studies; Lake Ontario field data, Oliver & Niimi 1985)
2.60, 2.48 (human fat of lipid, wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
5.32 (guppy, Gobas et al. 1987)
4.57 (*Selenastrum capricornutum*, Mailhot 1987)
4.48 (worms, Oliver 1987c)
4.84, 5.32 (fish, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)

3.85 (*Hexagenia limbata*, 4°C, rate const. ratio: uptake and depuration k_1/k_2, Landrum & Poore 1988)
4.94–5.28 (*Hexagenia limbata*, May-November, calculated-lipid-normalized, Landrum & Poore 1988)
5.01 (*Pontoporeia hoyi*, calculated, Evans & Landrum 1989)
5.06 (guppy, estimated, Banerjee & Baughman 1991)
5.65; 7.18 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
3.31–5.57 (various marine species, mean dry wt. BCF, Hope et al. 1998)
5.11–6.96 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.32 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
4.68, 5.93 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.48, 7.40 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.63, 6.99 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.65, 7.19 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.95; 3.95 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)
4.40 (estimated-EPIWIN v3.04, Hardy 2002)

Sorption Partition Coefficient, log K_P:
3.95–4.17 (Saginaw Bay sediment, sorption isotherm, Horzempa & Di Toro 1983)
4.12–4.55 (Saginaw Bay suspended solids, sorption isotherm, Horzempa & Di Toro 1983)
5.30 (Lake Superior suspended solids, field measurement-GC/ECD, Baker et al. 1986)
5.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.65–5.91 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
5.62 (soil/sediment, batch equilibrium-sorption isotherm, Haque & Schmedding 1976)
5.34 (soil, batch equilibrium-sorption isotherm measurement, Chiou et al. 1979)
6.51 (soil, calculated-K_{OW}, Karickhoff et al. 1979)
6.08 (soil, quoted experimental value, Kenaga 1980)
5.33 (calculated-K_{OW}, Schwarzenbach & Westall 1981)
6.51 (calculated-K_{OW}, Schwarzenbach & Westall 1981 from Karickhoff 1981)
6.43, 6.42, 5.33 (calculated-K_{OW}, calculated-C_L, calculated-C_S, Karickhoff 1981)
6.51 (sediment, calculated-K_{OW}, Lynch et al. 1982)
6.57 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.60; 5.50; 7.30 (field data of sediment trap material; Niagara River-org. matter; calculated-K_{OW}, Oliver & Charlton 1984)
6.61 (sediment/pore water-Saginaw Bay, dual radio-tag experiment, Di Toro et al. 1985)
5.51 (Aldrich humic acid, reversed phase separation, Landrum et al. 1985)
5.40, 5.70, 6.10 (Offshore Grand Haven sediment, nearshore Grand Haven sediment, Benton Harbor sediment, by batch equilibrium-sorption isotherm, Voice & Weber 1985)
7.56, 7.68 (river sediment, Coates & Elzerman 1986)
5.575 (correlated literature values in soils, Sklarew & Girvin 1987)
5.8–7.3, 6.60; 7.20 (suspended sediment, average; algae > 50 µm, Oliver 1987a)
6.60 (river sediment 7–13% OC, batch equilibrium, Oliver 1987)
6.48 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.75 (12 lakes/streams in southern Ontario at 1.6–26.5 mg/L DOC, Evans 1988)
5.26, 5.25, 5.19, 4.62 (humic substances, in concentration of 5, 10, 20, 40 mg/L DOC, reported as log K_h, Lara & Ernst 1989)
5.258, 5.222 (marine humic substances, calculated-MCI χ, reported as log K_h at concentration of 5 mg/L DOC, Sabljic et al. 1989)
6.76, 4.42 (Great Lake suspended matter, Great Lake DOC: reversed phase separation, Eadie et al. 1990)
6.18, 6.13, 5.99 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.86 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.54 (Red Hood sediment, batch equilibrium, Brannon et al. 1995)

5.65 (soil, calculated-MCI χ, Sabljic et al. 1995)
6.02 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
6.42–6.48 (Catlin silt loam, f_{OC} = 0.0226, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.77–6.84 (Cloudland loam, f_{OC} = 0.0024, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997
6.43–6.52 (Kenoma silt loam, f_{OC} = 0.0153, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.51–6.57 (Kenoma silt loam, f_{OC} = 0.0092, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.19–6.28 (Norborne silt loam, f_{OC} = 0.0137, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.55 (Norborne silt loam, f_{OC} = 0.009, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.41–6.59 (Norborne silt loam, f_{OC} = 0.0057, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.40 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.20; 5.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
5.86, 5.81 (sediments: organic carbon OC –0.1%, OC –0.5%, average, Delle Site 2001)
6.05–7.27; 5.30–7.60 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.55; 6.17, 6.96, 6.50 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
5.088 (estimated-EPIWIN v3.04, Hardy 2002)
6.20–7.20 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Sorption Partition Coefficient, log K_{OM}:
4.42 (natural sediment, Eadie et al. 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: depletion rate constant k = 17 d^{-1} from a 26-cm or 67-cm high purge vessel (Girvin et al. 1997); $t_{½}$ = 2.096 d from river, $t_{½}$ = 29.5 d from lake (estimated-EPIWIN v3.04, Hardy 2002).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16–0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 29.5 d^{-1} in pond, k_1 = 14.6 d^{-1} in river, k_1 = 36.8 d^{-1} in sand by *Chironomus tentans* larvae (Muir et al. 1983)
k_2 = 0.0029 d^{-1} with elimination $t_{½}$ = 241 h in pond-sediment, k_2 = 0.0059 d^{-1} with $t_{½}$ = 117 h in river water, k_2 = 0.0034 d^{-1} with $t_{½}$ = 203 h in river sediment and k_2 = 0.0030 d^{-1} with $t_{½}$ = 230 h in sand-sediment by *Chironomus tentans* larvae (Muir et al. 1983)
$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 800 d^{-1}; k_2 = 0.004 d^{-1} (guppy, Bruggeman et al. 1984)
k_1 = 461 d^{-1}; k_2 = 0.008 d^{-1} (rainbow trout, total ^{14}C in whole fish-wet weight, Muir et al. 1985)
k_1 = 1100 d^{-1} (guppy, Opperhuizen 1986)
k_1 = 63.2 h^{-1}; k_2 = 0.009 h^{-1} (10–20°C, *Hexagenia limbata*, Landrum & Poore 1988)
k_s = 0.049 h^{-1}; k_t = 0.009 h^{-1} (uptake, depuration of mayfly-sediment model II, Gobas et al. 1989)
log k_1 = 2.90, 2.66 d^{-1}; log $1/k_2$ = 2.39, 2.10 d (fish, quoted, Connell & Hawker 1990)
k_1 = 4660 d^{-1}; k_2 = 0.0104 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.044 d^{-1} with an elimination half-life of 15.9 d (earthworm, Belfroid et al. 1995)
k_2 = 0.003 d^{-1} with $t_{½}$ = 224 d and k_2 = 0.010 d^{-1} with $t_{½}$ = 69 d for food concn of 22 ng/g and 124 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_1 = 5.7 L d^{-1} g^{-1}; k_2 = 0.027 d^{-1} (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)
k_1 = 0.00231 h^{-1}; k_2 = 0.137 h^{-1} (in blood plasma of ring doves, Drouillard & Norstrom 2000)

k_1 = 5 (food lipid mg)/(g worm lipid-d); k_2 = 0.04 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{1/2}$ = 177 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{1/2}$ = 219 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
k_2 = 0.015 d^{-1} with $t_{1/2}$ = 46.2 d (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radical for hexachlorobiphenyls (Kwok et al. 1995);
$t_{1/2}$ = 6000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: 25–53 min in aqueous solution purged at a flow rate of 1 L/min (Coates 1984);
$t_{1/2}$ = 123000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000;
volatilization $t_{1/2}$ = 2.096 d from river, 29.5 d from lake (estimated-EPIWIN v3.04, Hardy 2002).

Groundwater:

Sediment: uptake clearance from sediment was (0.0021 ± 0.001) g of dry sediment·g^{-1} of organism·h^{-1} for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C (Landrum 1989);
k(exptl) < 0.9 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.7–6.3, with $t_{1/2}$ > 7 h at pH 7 and 23 ± 2°C (Yao & Haag 1991).
$t_{1/2}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: half-life in rainbow trout, > 1000 d and its muscle, 77 d (Niimi & Oliver 1983);
$t_{1/2}$ = 170 d in worms at 8°C (Oliver 1987c);
$t_{1/2}$ = 175 d in guppy (Bruggeman et al. 1984);
$t_{1/2}$ = 45.6 d in *Pontoporeia hoyi* (Evans & Landrum 1989);
elimination $t_{1/2}$ = 15.9 d from earthworm (Belfroid et al. 1995)
Depuration $t_{1/2}$ = 69–224 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
theoretical $t_{1/2}$ = 25.7 d to reach 90% steady-state tissue concn (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);
$t_{1/2}$ = 5.1 h in blood plasma (ring doves, Drouillard & Norstrom 2000);
elimination $t_{1/2}$ = 18 d in earthworm given contaminated food (Wågman et al. 2001).
depuration $t_{1/2}$ = 177 d for high-dose treatment, $t_{1/2}$ = 219 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
depuration $t_{1/2}$ = 46.2 d (juvenile carp in 100-d experiment Stapleton et al. 2004)

TABLE 7.1.1.153.1

Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,2′,4,4′,5,5′-hexachlorobiphenyl (PCB-153) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Doucette & Andren 1988		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	$S/g \cdot m^{-3}$	t/°C	$H/(Pa\ m^3/mol)$	t/°C	log K_{OA}
4	0.00462	4	6.50	–10	11.73
25	0.00845	11	13.52	0	11.25
40	0.0128	18	27.2	10	10.62
		25	52.8	20	10.04
$S/(mol/L) = A \cdot \exp[B \cdot (t/°C)]$		31	91.2	30	9.39
A	1.15×10^{-8}				
B	0.028	$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(kJ\ mol^{-1}) = 89.90$	
		A	22.8530		
$\Delta H_{sol}/(kJ\ mol^{-1}) = 20.3$		B	7950.45	log $K_{OA} = A + B/T$	
for 4–40°C				A	–6.015
		enthalpy, entropy change:		B	4695
		$\Delta H/(kJ \cdot mol^{-1}) = 66.1 \pm 5.4$			
		$\Delta S/(J \cdot mol^{-1} \cdot K^{-1}) = 190 \pm 18$			

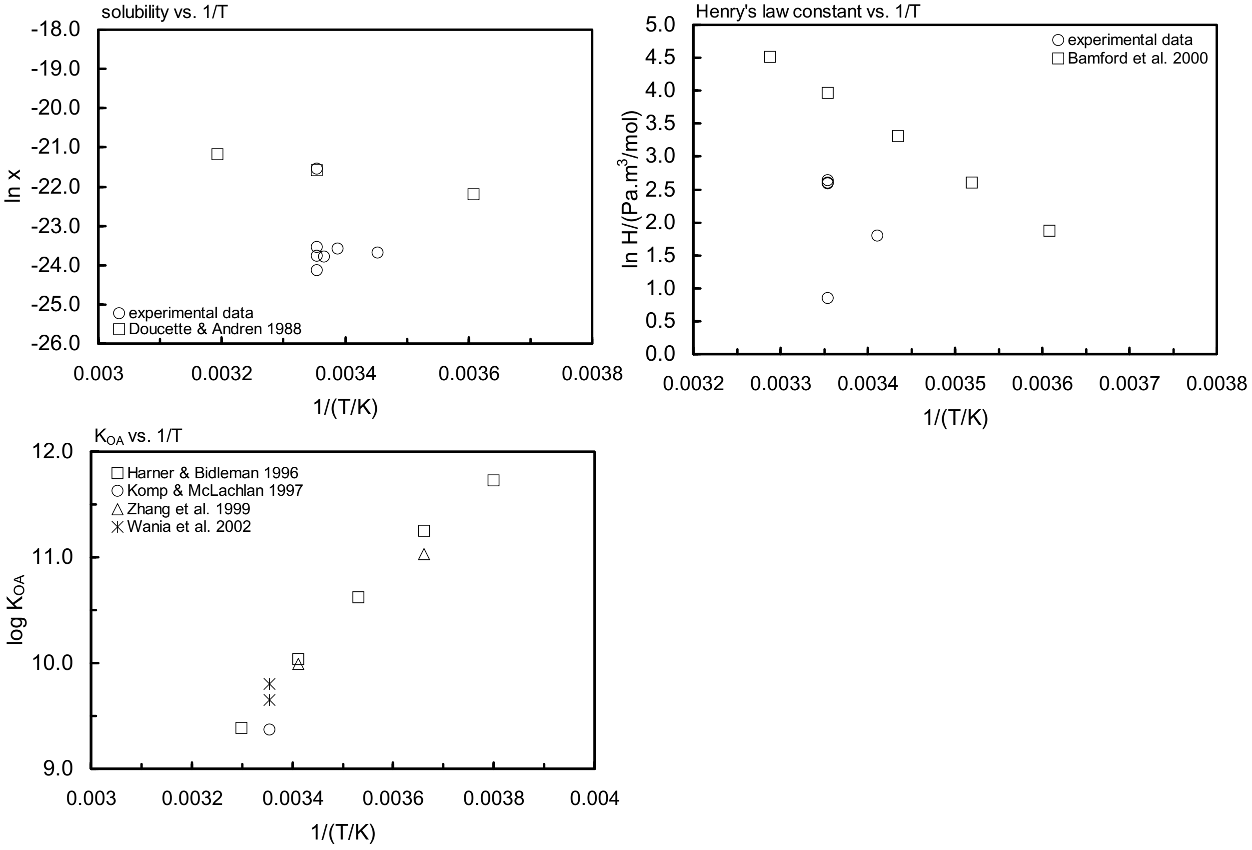
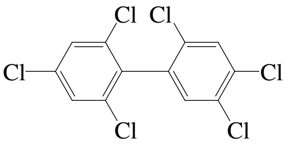


FIGURE 7.1.1.153.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,2′,4,4′,5,5′-hexachlorobiphenyl (PCB-153).

7.1.1.154 2,2′,4,4′,5,6′-Hexachlorobiphenyl (PCB-154)



Common Name: 2,2′,4,4′,5,6′-Hexachlorobiphenyl
Synonym: PCB-154, 2,2′,4,4′,5,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,5,6′-hexachlorobiphenyl
CAS Registry No: 60145-22-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
oil (Erickson 1986)
117 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
0.0106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00173, 0.00137, 0.00293, 0.00213 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.71×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.86×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
0.00182 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4681/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\cdot m^3/mol$ at 25°C or as indicated and reported temperature dependence equations):
58.46 (calculated-P/C, Burkhard 1984)
48.84 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
38.7 (calculated-QSPR, Dunnivant et al. 1992)
17.34, 29.16, 47.85, 76.7 ± 2.2, 113.7 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 15.155 - 5556.89/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(46.2/kJ\cdot mol^{-1})/RT] + (0.126/kJ\cdot mol^{-1}\cdot K^{-1})/R]$; where $R = 8.314\ J\cdot K^{-1}\cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
75.4 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 5$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.87 (calculated-TSA, Burkhard 1984)
6.67, 6.81, 6.47, 6.64 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.76 (calculated-TSA, Hawker & Connell 1988a)
7.05, 7.03; 6.48, 6.43 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.65	(recommended, Sangster 1993)
6.89	(recommended, Hansch et al. 1995)
6.6326	(molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

9.91	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.66	(suspended particulate matter, Burkhard 1984)
5.064	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16–0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

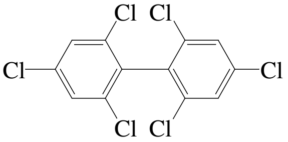
Ground water:

Sediment:

Soil:

Biota:

7.1.1.155 2,2′,4,4′,6,6′-Hexachlorobiphenyl (PCB-155)



Common Name: 2,2′,4,4′,6,6′-Hexachlorobiphenyl
Synonym: PCB-155, 2,2′,4,4′,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,6,6′-hexachlorobiphenyl
CAS Registry No: 33979-03-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
112.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3482
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.5 (differential scanning calorimetry, Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)
20.30 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
45.19 (Miller et al. 1984)
45.25, 66.9 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.139 (mp at 112.5°C)
0.131 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00090 (generator column-GC/ECD, Weil et al. 1974)
0.00041 (generator column-GC/ECD, Miller et al. 1984,1985)
0.0000528 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
2.50×10^{-3}, 1.34×10^{-3}, 6.27×10^{-3}, 2.68×10^{-3} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0023 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.00109 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
0.0033 (generator column-GC/ECD, Li et al. 1992; Li & Doucette 1993)
0.00284 (shake flask-GC/ECD, Li & Andren 1994)
0.0028* ± 0.00013 (generator column-GC/ECD, Shiu et al. 1997)
1.89×10^{-3}, 0.0050 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
$\ln x = -8.9206 - 4112.07/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0142, 0.0138 (supercooled liquid S_L: derivation of literature-derived value LDV, final-adjusted value FAV, Li et al. 2003)
$\log [S_L/(mol\ m^{-3})] = -861/(T/K) - 1.52$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log [S_L/(mol\ m^{-3})] = -1268/(T/K) - 0.16$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0016 (GC-RT, Westcott et al. 1981)
0.0122 (P_L calculated from P_S using fugacity ratio F, Westcott et al. 1981)
0.00173 (gas saturation, Westcott & Bidleman 1981)
0.00443 (supercooled liquid P_L, Burkhard 1984)

3.57×10^{-4}, 6.41×10^{-4}, 8.04×10^{-4} (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00443 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00159, 0.012(selected P_S, P_L, Shiu & Mackay 1986)
4.76×10^{-4} (calculated-S × HLC, Dunnivant & Elzerman 1988)
3.54×10^{-4} (supercooled liquid P_L, calculated-mp, Dunnivant & Elzerman 1988)
$\log (P_L/Pa) = -4303/(T/K) + 12.02$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
3.25×10^{-4}* (gas saturation-GC/ECD, measured range –10 to 30°C, Wania et al. 1994)
$\log (P_S/Pa) = 14.84 - 5399/(T/K)$; temp range –10 to 30°C (gas saturation-GC, Wania et al. 1994)
2.188×10^{-3} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
0.000285–0.0016; 0.00344–0.00443 (exptl. solid P_S range; exptl. liquid P_L range, Delle Site 1997)
3.42×10^{-4} (supercooled P_L: calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
3.31×10^{-3}; 3.47×10^{-3} (supercooled P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/Pa = -4697/(T/K) + 13.27$ (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
$\log P_L/Pa = -4562/(T/K) + 12.85$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

11.65 (gas stripping-GC, Coates 1984)
157.0 (calculated-P/C, Burkhard et al. 1985b)
12.46 (calculated, Coates & Elzerman 1986)
817.9 (calculated-P/C, Shiu & Mackay 1986)
76.5 (gas stripping-GC, Dunnivant et al. 1988, Dunnivant & Elzerman 1988)
60.8 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
85.25 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
75.86, 91.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -3294/(T/K) + 13.01$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

6.70 (shake flask-GC, Chiou et al. 1977)
6.34 (shake flask-GC, Karickhoff et al. 1979)
6.37 (HPLC-k′ correlation, McDuffie 1981)
7.12 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.88 (calculated-TSA, Burkhard 1984)
7.55 (generator column-GC/ECD, Miller et al. 1984,1985)
6.39 (HPLC-RT/MS correlation, Burkhard et al. 1985c)
6.01 (HPLC-k′ correlation, Tomlinson & Hafkenscheid 1986)
7.24 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
6.54, 6.81, 6.24, 6.57 (RP-HPLC-RI correlations, Brodsky & Ballschmiter 1988)
7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
7.287 ± 0.065(slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
7.08, 7.03; 6.24, 6.22 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.83 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
7.24 (shake flask-GC/ECD, Li & Doucette 1993)
6.54 (recommended, Sangster 1993)
7.29 (recommended, Hansch et al. 1995)
7.36, 7.19 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.99* (generator column-GC/ECD; measured range –10 to +20°C; Harner & Mackay 1995)
$\log K_{OA} = -2.20 + 3954/(T/K)$; (temp range –10 to +20°C, generator column-GC, Harner & Mackay 1995)

9.15 (20°C, generator column-GC, Harner & Bidleman 1996)
$\log K_{OA} = -2.21 + 3954/(T/K)$; temp range –10 to +20°C (generator column-GC, Harner & Bidleman 1996)
10.19, 9.13; 9.16 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.24 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.89, 9.14 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4357/(T/K) - 5.47$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:
1.02 (poultry, Garten & Trabalka 1983)
2.79–3.68 highest value 3.68, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7-d to 96-d laboratory study, Oliver & Niimi 1985)
> 4.94; 3.68 (rainbow trout, laboratory data: kinetic BCF (k_1/k_2), steady-state BCF (C_F/C_W), Oliver & Niimi 1985)
4.53 (worms, Oliver 1987c)
3.68 (fish, Isnard & Lambert 1988)
5.99, 7.29 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
6.08 (natural sediment, sorption isotherm by batch equilibrium technique-GC, Karickhoff et al. 1979)
5.95, 7.28, 5.95(calculated-K_{OW}, calculated-C_L, calculated-C_S, Karickhoff 1981)
6.68 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.905 (calculated-MCI χ, marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, Sabljic et al. 1989)
6.08; 6.17 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 8.6–29.5\ h^{-1}$ in pond-sediment system, $k_1 = 22.9–14.6\ h^{-1}$ in river-water system, $k_1 = 29.6–39.8\ h^{-1}$ in river-send system, $k_1 = 26.7–47.0\ h^{-1}$ in sand-sediment system (*Chironomus tentans* larvae, Muir et al. 1983)
$k_2 = 0.0029\ h^{-1}$ with $t_{½} = 241$ h in pond-sediment system, $k_2 = 0.0059\ h^{-1}$ with $t_{½} = 117$ h in river-water system, $k_2 = 0.0034\ h^{-1}$ with $t_{½} = 203$ h in river-send system, $k_2 = 0.0030\ h^{-1}$ with $t_{½} = 230$ h in sand-sediment system (*Chironomus tentans* larvae, Muir et al. 1983)
$k_2 > 0.0007\ d^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 60\ d^{-1}$; $k_2 > 0.0007\ d^{-1}$ (rainbow trout, Oliver & Niimi 1985; Thomann 1989)
$\log 1/k_2 = 3.1, 3.6$ h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)
$1/k_2 = 141$ d (guppy, Gobas et al. 1989; quoted, Clark et al. 1990)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:

Biota: $t_{1/2}$ = 117–241 h in sediment-water systems (*Chironomus tentans* larvae, Muir et al. 1983)
$t_{1/2}$ > 1000 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{1/2}$ = 77 d in its muscle (Niimi & Oliver 1983).

TABLE 7.1.1.155.1
Reported aqueous solubilities and octanol-air partition coefficients log of 2,2′,4,4′,6,6′-hexachlorobiphenyl (PCB-155) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1997		Wania et al. 1994		Harner & Mackay 1995	
generator column-GC/ECD		gas saturation-GC		generator column-GC	
t/°C	$S/g\cdot m^{-3}$	t/°C	P/Pa	t/°C	log K_{OA}
5	1.0×10^{-3}	–10	1.634×10^{-6}	–10	10.49
15	1.70×10^{-3}	0	1.185×10^{-5}	0	9.97
25	2.80×10^{-3}	10	8.039×10^{-5}	10	9.635
35	4.30×10^{-3}	20	3.250×10^{-4}	20	9.158
45	6.40×10^{-3}	30	7.739×10^{-4}	25	8.99
$\Delta H_{sol}/(kJ\ mol^{-1}) = 34.2$		log (P/Pa) = A – B/(T/K)		$\Delta H_{OA}/(kJ\ mol^{-1}) = 63.9$	
for 5–45°C		A	14.84		
		B	5399	log K_{OA} = A + B/RT	
				A	–2.2
		$\Delta H_{subl}/(kJ\ mol^{-1}) = 103.4$		B	3337.4

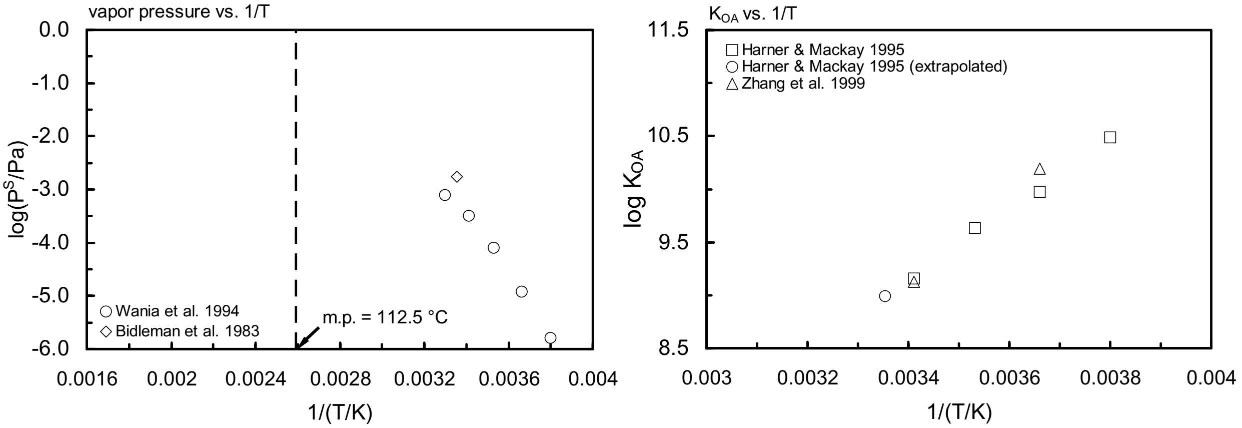
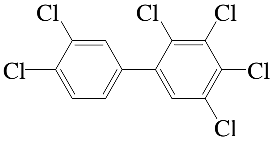


FIGURE 7.1.1.155.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 2,2′,4,4′,6,6′-hexachlorobiphenyl (PCB-155).

7.1.1.156 2,3,3′,4,4′,5-Hexachlorobiphenyl (PCB-156)



Common Name: 2,3,3′,4,4′,5-Hexachlorobiphenyl
Synonym: PCB-156, 2,3,3′,4,4′,5-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5-hexachlorobiphenyl
CAS Registry No: 38380-08-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
  127 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  310.0 (calculated-Le Bas method at normal boiling point)
  237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F: 0.100 (mp at 127°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  0.00533 (20°C, supercooled liquid S_L, Murphy et al. 1987)
  0.00361, 0.00244, 0.00112, 0.00102 (RP-HPLC-k′ correlation, different stationary and mobile phases Brodsky & Ballschmiter 1988)
  0.000397 (generator column-GC/ECD, Hong & Qiao 1995)
  0.0011 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
  0.000513, 0.000711, 0.00110, 0.00153 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.000215 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
  7.34×10^{-4} (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985a)
  0.000809 (GC-RI correlation, Burkhard et al. 1985b)
  0.00021, 0.00016 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  1.26×10^{-4}, 1.62×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
  $\log (P_L/\text{Pa}) = -4949/(T/\text{K}) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  88.14 (concn ratio-GC, Murphy & Mullin 1983)
  17.53 (calculated-P/C, Burkhard et al. 1985)
  2.23 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  8.97 (calculated-QSPR, Dunnivant et al. 1992)
  1.50 (calculated-QSPR, Achman et al. 1993)
  3.72 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  37.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 112 \pm 10$ kJ/mol, $\Delta S_H = 0.34 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.13, 7,26, 7.84, 7.53 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.14, 7.12; 7.16, 7.13 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.70 (generator column-GC, Larsen et al. 1992)
7.11 (recommended, Sangster 1993)
7.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.07, 10.87; 10.87 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.36 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.88, 7.18 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.51 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.40 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)

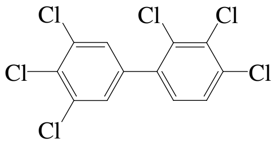
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.024 d^{-1} with an elimination $t_{½}$ = 29 d (earthworm, Belfroid et al. 1995)
k_2 = 0.004 d^{-1} with $t_{½}$ = 163 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 182 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: clearance $t_{½}$ = 50–100 d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);
reported biological half-lives for hexachlorobiphenyls: $t_{½}$ = 87 to > 850 d for trout, $t_{½}$ = 77–91 d for trout muscle; $t_{½}$ > 200 d for carp; $t_{½}$ = 75–175 d for guppy (Niimi 1987);
elimination $t_{½}$ = 29 d from earthworm (Belfroid et al. 1995)
depuration $t_{½}$ = 163 d for high-dose treatment, $t_{½}$ = 182 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.157 2,3,3′,4,4′,5′-Hexachlorobiphenyl (PCB-157)



Common Name: 2,3,3′,4,4′,5′-Hexachlorobiphenyl
Synonym: PCB-157, 2,3,3′,4,4′,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5′-hexachlorobiphenyl
CAS Registry No: 69782-90-7
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
141 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0152 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00036 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.000119 (generator column-GC/ECD, Hong & Qiao 1995)
0.000296 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000084, 0.000139, 0.000296, 0.000540 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.39×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
8.09×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
2.02×10^{-4}, 1.27×10^{-4} (supercooled liquid P_L, GC-RT correlation; different stationary phases, Foreman & Bidleman 1985)
1.17×10^{-4}, 1.58×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4994/(T/K) + 13.05$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
3.30 (calculated-P/C, Burkhard et al. 1985a)
58.76 (concn ratio-GC, Murphy & Mullin 1983)
6.69 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
8.56 (calculated-QSPR, Dunnivant et al. 1992)
1.50 (calculated-QSPR, Achman et al. 1993)
2.27 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
31.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 129 \pm 10$ kJ/mol, $\Delta S_H = 0.40 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.18 (calculated-TSA, Hawker & Connell 1988a)
7.26, 7.14; 7.19, 7.04 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.20 (quoted average values of Risby et al. 1990: GC-RV and HPLC-k′ correlations, Sangster 1993)

7.60 (recommended, Hansch et al. 1995)
6.9661 (calculated-molecular properties MNDO-AM1, Makino 1998)
6.73; 6.90 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
7.37, 6.97 (calculated-MCI χ, calculated-MNDO-AMI method, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.28, 11.07; 10.76 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.57 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.51 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.40 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)

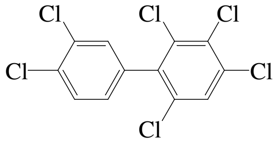
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: clearance $t_{1/2}$ = 50–100 d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);
reported biological half-lives for hexachlorobiphenyls: $t_{1/2}$ = 87 to > 850 d for trout, $t_{1/2}$ = 77–91 d for trout muscle; $t_{1/2}$ > 200 d for carp; $t_{1/2}$ = 75–175 d for guppy (Niimi 1987)

7.1.1.158 2,3,3′,4,4′,6-Hexachlorobiphenyl (PCB-158)



Common Name: 2,3,3′,4,4′,6-Hexachlorobiphenyl
Synonym: PCB-158, 2,3,3′,4,4′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,6-hexachlorobiphenyl
CAS Registry No: 74472-42-7
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
107 (Kühne et al. 1995; Ruelle & Kesselring 1997; Ran et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.157 (mp at 107°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0159 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00807 (20°C, supercooled liquid, Murphy et al. 1987)
0.00120 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00114 (TSA and mp, Abramowitz & Yalkowsky 1990)
0.00185 (calculated-group contribution method, Kühne et al. 1995)
0.00147, 0.00396 (molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
9.26×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.02×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
6.19×10^{-4}, 4.486×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.73×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
3.09×10^{-4}, 4.57×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4816/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
20.97 (calculated-P/C, Burkhard 1984)
4.37 (20°C, calculated-P/C, Murphy et al. 1987)
21.89 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.86 (calculated-QSPR, Achman et al. 1993)
16.74 (calculated-QSPR, Dunnivant et al. 1992)
9.64 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 80 \pm 7$ kJ/mol, $\Delta S_H = 0.24 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.69	(calculated-TSA, Burkhard 1984)
6.78	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.02	(calculated-TSA, Hawker & Connell 1988a)
7.10, 6.87; 6.84, 6.82	(multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.78	(recommended, Sangster 1993)
7.25	(recommended, Hansch et al. 1995)
6.8874	(calculated-molecular properties MNDO-AM1 method, Makino 1998)
7.69	(calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

9.51; 9.12 (generator column-GC.; K_{OW}/K_{AW}, Kömp & McLachlan 1997a)

$K_{OA} = -5.17 + 4380/(T/K)$, temp range 10–43°C (Kömp & McLachlan 1997a)

10.28 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.49	(suspended particulate matter, Burkhard 1984)
5.241	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc)$ = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.006$ d^{-1} with $t_{½}$ = 124 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d^{-1} with $t_{½}$ = 241 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

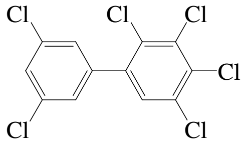
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 124 d for high-dose treatment, $t_{½}$ = 241 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.159 2,3,3′,4,5,5′-Hexachlorobiphenyl (PCB-159)



Common Name: 2,3,3′,4,5,5′-Hexachlorobiphenyl
Synonym: PCB-159, 2,3,3′,4,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5,5′-hexachlorobiphenyl
CAS Registry No: 39635-35-3
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
116 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0135 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
5.72×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.084×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00119 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
29.08 (calculated-P/C, Burkhard 1984)
31.41 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.027 (wetted wall column-GC/ECD, Brunner et al. 1990)
15.77 (calculated-QSPR, Dunnivant et al. 1992)
35.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 116 \pm 12$ kJ/mol, $\Delta S_H = 0.35 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
7.24 (calculated-TSA, Hawker & Connell 1988a)
7.09, 7.24; 7.02, 7.00 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.17, 7.01 (quoted average values of Risby et al. 1990, Sangster 1993)
7.43 (recommended, Hansch et al. 1995)
7.2038 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.37 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.56	(suspended particulate matter, Burkhard 1984)
5.381	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

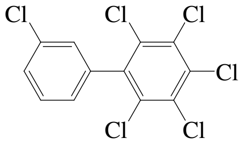
Ground water:

Sediment:

Soil:

Biota:

7.1.1.160 2,3,3′,4,5,6-Hexachlorobiphenyl (PCB-160)



Common Name: 2,3,3′,4,5,6-Hexachlorobiphenyl
Synonym: PCB-160, 2,3,3′,4,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5,6-hexachlorobiphenyl
CAS Registry No: 41411-62-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
99 (Burkhard et al. 1985b)
97–100 (Erickson 1986)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.188 (mp at 99°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0191 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00158 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
1.33×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00027 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
25.13 (calculated-P/C, Burkhard 1984)
25.74 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.027 (wetted wall column-GC/ECD, Brunner et al. 1990)
21.66 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.62 (calculated-TSA, Burkhard 1984)
6.93 (calculated-TSA, Hawker & Connell 1988a)
6.88, 6.79; 6.89, 6.87 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.84, 6.88 (quoted average values of Risby et al. 1990, Sangster 1993)
7.30 (recommended, Hansch et al. 1995)
6.9006 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.42	(suspended particulate matter, Burkhard 1984)
5.259	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

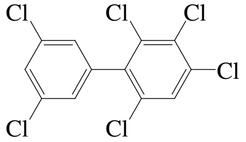
Ground water:

Sediment:

Soil:

Biota:

7.1.1.161 2,3,3′,4,5′,6-Hexachlorobiphenyl (PCB-161)



Common Name: 2,3,3′,4,5′,6-Hexachlorobiphenyl
Synonym: PCB-161, 2,3,3′,4,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5′,6-hexachlorobiphenyl
CAS Registry No: 74472-43-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
  84.0 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
  0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
  1.37×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.00150 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  34.96 (calculated-P/C, Burkhard 1984)
  51.27 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  28.89 (calculated-QSPR, Dunnivant et al. 1992)
  49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  6.76 (calculated-TSA, Burkhard 1984)
  7.08 (calculated-TSA, Hawker & Connell 1988a)
  7.16, 6.94; 6.69, 6.66 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
  7.05, 6.68 (quoted average values of Risby et al. 1990, Sangster 1993)
  7.10 (recommended, Hansch et al. 1995)
  7.0318 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
  10.33 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.56	(suspended particulate matter, Burkhard 1984)
5.222	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.16 – 0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

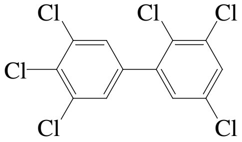
Ground water:

Sediment:

Soil:

Biota:

7.1.1.162 2,3,3′,4′,5,5′-Hexachlorobiphenyl (PCB-162)



Common Name: 2,3,3′,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-162, 2,3,3′,4,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 39635-34-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
84.0 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.37×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00150 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
34.96 (calculated-P/C, Burkhard 1984)
51.27 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
28.89 (calculated-QSPR, Dunnivant et al. 1992)
35.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 116 \pm 12$ kJ/mol, $\Delta S_H = 0.35 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
7.08 (calculated-TSA, Hawker & Connell 1988a)
7.16, 6.94; 6.69, 6.66 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.05, 6.68 (quoted average values of Risby et al. 1990, Sangster 1993)
7.10 (recommended, Hansch et al. 1995)
7.0318 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.42 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.56	(suspended particulate matter, Burkhard 1984)
5.222	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

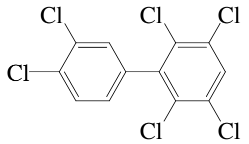
Ground water:

Sediment:

Soil:

Biota:

7.1.1.163 2,3,3′,4′,5,6-Hexachlorobiphenyl (PCB-163)



Common Name: 2,3,3′,4′,5,6-Hexachlorobiphenyl
Synonym: PCB-163, 2,3,3′,4′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5,6-hexachlorobiphenyl
CAS Registry No: 74472-44-9
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
88.2 (Shiu & Mackay 1986)
122 (Ran et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.237 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.00531 (generator column-HPLC/UV, Huang 1983)
0.0053 (generator column-HPLC/UV, Billington et al. 1988)
0.0012 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
8.67×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.54×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
6.01×10^{-4}, 4.92×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.31×10^{-4}, 5.25×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4816/(T/\text{K}) + 12.93$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
18.54 (calculated-P/C, Burkhard 1984)
11.75 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
1.52 (wetted wall column-GC/ECD, Brunner et al. 1990)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
9.37 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 81 \pm 7$ kJ/mol, $\Delta S_H = 0.24 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.78 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.08; 6.99; 6.84, 6.79 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.39 (generator column-GC, average, Larsen et al. 1992)
6.78 (recommended, Sangster 1993)
7.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.26, 10.16	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.90	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.47	(suspended particulate matter, Burkhard 1984)
5.241	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004$ d^{-1} with $t_{½} = 170$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d^{-1} with $t_{½} = 198$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

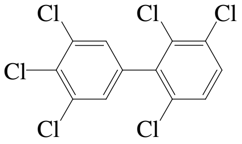
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 170 d for high-dose treatment, $t_{½}$ = 198 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.164 2,3,3′,4′,5′,6-Hexachlorobiphenyl (PCB-164)



Common Name: 2,3,3′,4′,5′,6-Hexachlorobiphenyl
Synonym: PCB-164, 2,3,3′,4′,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5′,6-hexachlorobiphenyl
CAS Registry No: 74472-45-0
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
 96 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
 310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
 0.0161 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
 0.00194 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 0.00144 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
 4.478×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
 4.97×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
 10.04 (calculated-P/C, Burkhard 1984)
 19.96 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
 17.41 (calculated-QSPR, Dunnivant et al. 1992)
 49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
 6.69 (calculated-TSA, Burkhard 1984)
 6.63 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 7.02 (calculated-TSA, Hawker & Connell 1988a)
 7.22, 7.32; 6.79, 6.73 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
 6.63 (recommended, Sangster 1993)
 7.20 (recommended, Hansch et al. 1995)
 6.6712 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
 10.35 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.49	(suspended particulate matter, Burkhard 1984)
5.241	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.16 – 0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

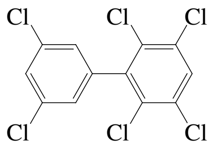
Ground water:

Sediment:

Soil:

Biota:

7.1.1.165 2,3,3′,5,5′,6-Hexachlorobiphenyl (PCB-165)



Common Name: 2,3,3′,5,5′,6-Hexachlorobiphenyl
Synonym: PCB-165, 2,3,3′,5,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5,5′,6-hexachlorobiphenyl
CAS Registry No: 74472-46-1
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
101 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0150 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00114 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.292×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00140 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
30.9 (calculated-P/C, Burkhard 1984)
45.19 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.94 (wetted wall column-GC/ECD, Brunner et al. 1990)
27.91 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.57, 7.37 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.72 (calculated-TSA, Burkhard 1984)
7.05 (calculated-TSA, Hawker & Connell 1988a)
7.17, 6.90; 6.70, 6,65 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.37, 6.68, 7.04 (quoted literature values, Sangster 1993)
7.37 (recommended, Hansch et al. 1995)
7.0191 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.88 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.52	(suspended particulate matter, Burkhard 1984)
5.222	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

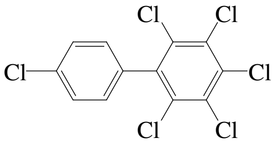
Ground water:

Sediment:

Soil:

Biota:

7.1.1.166 2,3,4,4′,5,6-Hexachlorobiphenyl (PCB-166)



Common Name: 2,3,4,4′,5,6-Hexachlorobiphenyl
Synonym: PCB-166, 2,3,4,4′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′,5,6-hexachlorobiphenyl
CAS Registry No: 41411-63-6
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
  163.0 (Burkhard et al. 1985b)
  160–165 (Erickson 1986)
  145 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0443 (mp at 163°C)

Water Solubility (g/m^3 or mg/L at 25°C):
  0.0189 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  7.20×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
  2.46×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
  1.175×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.00140 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  22.49 (calculated-P/C, Burkhard 1984)
  17.43 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  18.65 (calculated-QSPR, Dunnivant et al. 1992)
  49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  6.62 (calculated-TSA, Burkhard 1984)
  6.93 (calculated-TSA, Hawker & Connell 1988a)
  7.13, 7.18; 6.90, 6.83 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
  7.17, 6.87 (quoted average values of Risby et al. 1990, Sangster 1993)
  7.31 (recommended, Hansch et al. 1995)
  6.8501 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
  10.08 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.42 (suspended particulate matter, Burkhard 1984)

5.259 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

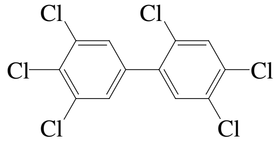
Ground water:

Sediment:

Soil:

Biota:

7.1.1.167 2,3′,4,4′,5,5′-Hexachlorobiphenyl (PCB-167)



Common Name: 2,3′,4,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-167, 2,3′,4,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 52663-72-6
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
  135 (calculated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  0.0128 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.00223 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  0.00036 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
  0.000531 (generator column-GC/ECD, Hong & Qiao 1995)
  0.000107 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
  0.000442, 0.000682, 0.00107, 0.00161 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  1.88×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  2.12×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
  2.80×10^{-4}, 2.39×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  2.34×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
  $\log (P_L/\text{Pa}) = -4994/(T/\text{K}) + 13.20$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  5.33 (calculated-P/C, Burkhard et al. 1985a)
  12.46 (calculated-QSPR-MCIχ, Sabljic & Güsten 1989)
  20.55 (calculated-QSPR, Dunnivant et al. 1992)
  4.47 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  39.28 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 106 \pm 8$ kJ/mol, $\Delta S_H = 0.32 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  7.29 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  7.24, 7.30; 7.00, 7.03 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
  7.29 (recommended, Sangster 1993)
  7.50 (recommended, Hansch et al. 1995)
  6.82 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or indicated:

12.07, 10.77; 10.76 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

10.59	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.97, 7.27	(fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.58	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.381	(as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.0263$ d^{-1} with an elimination $t_{½}$ = 26 4 d (earthworm, Belfroid et al. 1995)

$k_2 = 0.005$ d^{-1} with $t_{½}$ = 134 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005$ d^{-1} with $t_{½}$ = 153 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{½}$ = 38 min when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW Xenon lamp (De Felip et al. 1996)

Ground water:

Sediment:

Soil:

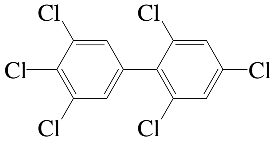
Biota: clearance $t_{½}$ = 50–100 d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);

reported biological half-lives for hexachlorobiphenyls: $t_{½}$ = 87 to > 850 d for trout, $t_{½}$ = 77–91 d for trout muscle; $t_{½}$ > 200 d for carp; $t_{½}$ = 75–175 d for guppy (Niimi 1987);

elimination $t_{½}$ = 26.4 d from earthworm (Belfroid et al. 1995)

depuration $t_{½}$ = 134 d for high-dose treatment, $t_{½}$ = 153 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.168 2,3′,4,4′,5′,6-Hexachlorobiphenyl (PCB-168)



Common Name: 2,3′,4,4′,5′,6-Hexachlorobiphenyl
Synonym: PCB-168, 2,3′,4,4′,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,5′,6-hexachlorobiphenyl
CAS Registry No: 59291-65-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
  110–111 (Erickson 1986)
  133 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
  0.0134 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  5.72×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
  9.76×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  4.87×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  5.40×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
  6.88×10^{-4}, 6.24×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  $\log (P_L/\text{Pa}) = -4816/(T/\text{K}) + 12.99$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):
  13.07 (calculated-P/C, Burkhard 1984)
  46.91 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
  27.97 (calculated-QSAR, Dunnivant et al. 1992)
  49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  6.76 (calculated-TSA, Burkhard 1984)
  7.11 (calculated-TSA, Hawker & Connell 1988a)
  7.23, 7.13; 6.76, 6.71 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
  7.18, 6.74 (quoted average values from Risby et al. 1990, Sangster 1993)
  7.17 (recommended, Hansch et al. 1995)
  6.8539 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

10.39 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.56 (suspended particulate matter, Burkhard 1984)

5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calc-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

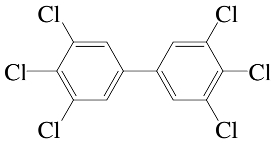
Ground water:

Sediment:

Soil:

Biota:

7.1.1.169 3,3′,4,4′,5,5′-Hexachlorobiphenyl (PCB-169)



Common Name: 3,3′,4,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-169, 3,3′,4,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 3,3′,4,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 32774-16-6
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
    201–202.0 (Hutzinger et al. 1974)
    201 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
    310.0 (calculated-Le Bas method at normal boiling point)
    237.4 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
    56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
    0.0178 (calculated, Mackay et al. 1992; Passivirta et al. 1999)
    0.0177 (Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
    4.54×10^{-4}, 3.0×10^{-4}, 5.22×10^{-4}, 9.07×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
    0.0000219; 0.000116 (generator column-GC, ECD; estimated, Hong & Qiao 1995)
    $\log (S_L/(\text{mol/L})) = -1.12 + 1403/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
    0.000130 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
    0.000053, 0.000083, 0.000130, 0.000215 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    1.08×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)
    5.36×10^{-5} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
    6.76×10^{-5} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
    $\log (P/_L/Pa) = - 5313/(T/K) + 13.64$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
    1.03×10^{-4}, 1.82×10^{-6} (supercooled liquid P_L, solid P_S, Passivirta et al. 1999)
    $\log (P_S/Pa) = 16.59 - 6715/(T/K)$ (solid, Passivirta et al. 1999)
    $\log (P_L/Pa) = 13.64 - 5313/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa m^3/mol at 25°C):
    1.57 (calculated-P/C, Burkhard et al. 1985b)
    5.98 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
    6.60 (calculated-QSPR, Dunnivant et al. 1992)
    0.85 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
    23.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
    $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 162 \pm 20$ kJ/mol, $\Delta S_H = 0.51 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.42, 7.54, 7.62, 7.61 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.408 ± 0.005 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)

7.39, 7.55; 7.46, 7.42 (multi-column HPLC-k′ correlation; capillary GC-RT correlation, different stationary phases, Risby et al. 1990)

7.55 (recommended, Sangster 1993)

7.41 (recommended, Hansch et al. 1995)

7.01 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or indicated:

12.51, 11.32; 11.19 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

11.27 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.97; 7.50 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

5.97, 7.51 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.60 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 7200\ d^{-1}$; $k_2 = 0.00766\ d^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_1 = 2 (food lipid mg)/(g worm lipid-d); $k_2 = 0.03\ d^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.0065\ d^{-1}$ with $t_{½}$ = 107 d (newly contaminated oysters, Gardinali et al. 2004)

$k_2 = 0.0082\ d^{-1}$ with $t_{½}$ = 85 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995);

$t_{½}$ = 6000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photodegradation $t_{½}$ = 548 min when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996);

$t_{½}$ = 120000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Groundwater:

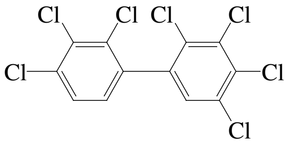
Sediment: $t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{½}$ = 24 d in earthworm given contaminated food (Wågman et al. 2001)

Depuration $t_{½}$ = 107 d for newly contaminated oysters, and $t_{½}$ = 85 d for chronically contaminated oysters (Gardinali et al. 2004)

7.1.1.170 2,2′,3,3′,4,4′,5-Heptachlorobiphenyl (PCB-170)



Common Name: 2,2′,3,3′,4,4′,5-Heptachlorobiphenyl
Synonym: PCB-170, 2,2′,3,3′,4,4′,5-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5-heptachlorobiphenyl
CAS Registry No: 35065-30-6
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
135 (Hutzinger et al. 1974; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0833 (mp at 135°C)

Water Solubility (g/m^3 or mg/L at 25°C):

0.00767	(supercooled liquid S_L, Burkhard et al. 1985b)
0.00347	(20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.000504	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.000395	(calculated-TSA, Abramowitz & Yalkowsky 1990)
0.00052	(calculated-MCI χ, Patil 1991)
0.000130	(calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

8.37×10^{-5} (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
3.37×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
3.72×10^{-4} (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
8.37×10^{-5}, 8.11×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.32×10^{-5} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
5.13×10^{-5}, 7.76×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5139/(T/\text{K}) + 13.07$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19.25 (calculated-P/C, Burkhard 1985b)
1.52 (20°C, calculated-P/C, Murphy et al. 1987)
0.912 (wetted-wall column-GC, Brunner et al. 1990)
8.85 (calculated-QSPR, Dunnivant et al. 1992)
0.128, 0.760, 4.139, 20.84* ± 0.80, 78.50 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 61.342 - 19725.76/(T/\text{K})$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(164.0/\text{kJ·mol}^{-1})/RT] + (0.510/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 $\text{J·K}^{-1}\text{·mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
19.4 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 164 ± 9 kJ/mol, ΔS_H = 0.51 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.05	(calculated-TSA, Burkhard 1984)
7.08	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.27	(calculated-TSA, Hawker & Connell 1988a)
7.03	(calculated-MCI χ, Patil 1991)
7.30	(calculated-TSA, Murray & Andren 1992)
6.83	(generator column-GC, Larsen et al. 1992)
6.96	(recommended, Sangster 1993)
7.10	(estimated, Girvin & Scott 1997)
7.0639	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.42	(10°C, estimated, Thomas et al. 1998)
12.34, 11.07; 11.02	(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.69	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

2.43–4.76	(various marine species, mean dry wt. BCF, Hope et al. 1998)
3.75–4.61	(Various marine species, mean lipid-normalized BCF, Hope et al. 1999)

Sorption Partition Coefficient, log K_{OC}:

6.85	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.63, 5.48, 5.42, 4.99	(marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.632, 5.675	(marine humic substances of 5 mg/L DOC, quoted; calculated-MCI χ, reported as association coefficient log K_h, Sabljic et al. 1989)
6.10	(colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.60	(soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 164$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 180$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

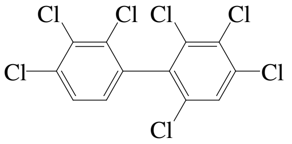
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 164 d for high-dose treatment, $t_{1/2}$ = 180 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.171 2,2′,3,3′,4,4′,6-Heptachlorobiphenyl (PCB-171)



Common Name: 2,2′,3,3′,4,4′,6-Heptachlorobiphenyl
Synonym: PCB-171, 2,2′,3,3′,4,4′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,6-heptachlorobiphenyl
CAS Registry No: 52663-71-5
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):

117.5	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

330.9	(calculated-Le Bas method at normal boiling point)
250.3	(Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.29	(Miller et al. 1984; Ruelle et al. 1993)
22.80	(Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

51.04	(Miller et al. 1984; Shiu & Mackay 1986)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.124 (mp at 117.5°C)

0.109	(Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.00624	(shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00217	(generator column-GC/ECD, Miller et al. 1984,1985)
0.00412	(20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
9.81×10^{-6}	(calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
0.00102, 0.000687, 0.000521	(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

1.87×10^{-4}, 2.98×10^{-4}	(supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
5.71×10^{-4}	(GC-RI correlation, Burkhard et al. 1985a)
4.69×10^{-4}	(supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
2.57×10^{-4}, 3.17×10^{-4}	(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.73×10^{-5}, 2.50×10^{-4}	(selected, solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
1.26×10^{-4}, 2.09×10^{-4}	(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5008/(T/K) + 13.07$	(supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
9.77×10^{-5}	(20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa m^3/mol at 25°C):

29.79	(calculated-P/C, Burkhard et al. 1985b)
5.40	(calculated-P/C, Shiu & Mackay 1986)
17.49	(calculated-QSPR, Dunnivant et al. 1992)
1.50	(calculated-QSPR, Achman et al. 1993)

59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (calculated-TSA, Burkhard 1984)
6.68 (generator column-GC/ECD, Miller et al. 1984,1985)
7.85 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
7.04, 7.06 (RP-HPLC-k′ correlation, different mobile phases, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.99 (recommended, Sangster 1993)
6.68 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
9.50 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
10.51 (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
12.31, 11.78, 11.14, 10.51, 9.96 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
log $K_{OA} = -5.71 + 4757/(T/K)$; (temp range –10 to 30°C, Harner & Bidleman 1996)
11.76, 10.51; 10.50 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.76 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

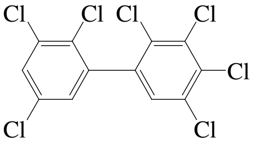
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
6.94 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.516 (marine humic substances of 5 mg/L DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.004$ d^{-1} with $t_{½} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½} = 182$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½} = 260$ d in worms at 8°C (Oliver 1987c).
depuration $t_{½} = 156$ d for high-dose treatment, $t_{½} = 182$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.172 2,2′,3,3′,4,5,5′-Heptachlorobiphenyl (PCB-172)



Common Name: 2,2′,3,3′,4,5,5′-Heptachlorobiphenyl
Synonym: PCB-172, 2,2′,3,3′,4,5,5′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′-heptachlorobiphenyl
CAS Registry No: 52663-74-8
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
113 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00688 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00430 (20°C, supercooled liquid, Murphy et al. 1987)
3.14×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
4.98×10^{-4} (calculated-TSA and mp., Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.55×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
6.14×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.41×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5109/(T/K) + 12.28$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
31.82 (calculated-P/C, Burkhard 1984)
1.317 (wetted wall column-GC/ECD, Brunner et al. 1990)
12.07 (calculated-QSPR, Dunnivant et al. 1992)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.10 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.85 (generator column-GC, Larsen et al. 1992)
7.33 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.03 (recommended, Sangster 1993)
7.2349 (molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.84, 10.67 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.50 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.89 (suspended particulate matter, Burkhard 1984)

5.71, 5.44, 5.38, 4.97 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)

5.711; 5.66 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 165$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 179$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

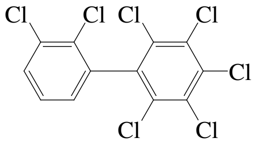
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½} = 165$ d for high-dose treatment, $t_{½} = 179$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.173 2,2′,3,3′,4,5,6-Heptachlorobiphenyl (PCB-173)



Common Name: 2,2′,3,3′,4,5,6-Heptachlorobiphenyl
Synonym: PCB-173, 2,2′,3,3′,4,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,6-heptachlorobiphenyl
CAS Registry No: 68194-16-1
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):

145	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

330.9	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.00731	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00416	(20°C, supercooled liquid, Murphy et al. 1987)
6.265×10^{-4}	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):

5.55×10^{-5}	(P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
6.14×10^{-4}	(GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):

29.89	(calculated-P/C, Burkhard 1984)
1.42	(wetted wall column-GC/ECD, Brunner et al. 1990)
18.48	(calculated-QSPR, Dunnivant et al. 1992)
59.9	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.07	(calculated-TSA, Burkhard 1984)
7.02	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.30	(calculated-TSA, Murray & Andren 1992)
6.9556	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.79, 10.60	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.48	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.87	(suspended particulate matter, Burkhard 1984)
5.532	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.40	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

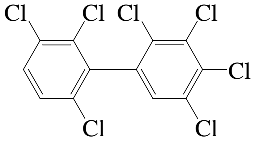
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 2 (food lipid mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{1/2}$ = 162 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{1/2}$ = 186 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{1/2}$ = 20 d in earthworm given contaminated food (Wågman et al. 2001)
depuration $t_{1/2}$ = 162 d for high-dose treatment, $t_{1/2}$ = 186 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.174 2,2′,3,3′,4,5,6′-Heptachlorobiphenyl (PCB-174)



Common Name: 2,2′,3,3′,4,5,6′-Heptachlorobiphenyl
Synonym: PCB-174, 2,2′,3,3′,4,5,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,6′-heptachlorobiphenyl
CAS Registry No: 38411-25-5
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
130.6 (Burkhard 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (KJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.092 (mp at 130.6°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00625 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00525 (20°C, supercooled liquid, Murphy et al. 1987)
0.001016 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.687×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
3.191×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.206×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.19×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.80×10^{-4}, 2.43×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
6.69×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
2.75×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4962/(T/\text{K}) + 12.90$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
93.53 (calculated-P/C, Burkhard 1984)
4.96 (20°C, calculated-P/C, Murphy et al. 1987)
1.419 (wetted wall column-GC/ECD, Brunner et al. 1990;)
17.13 (calculated-QSPR, Dunnivant et al. 1992)
4.91 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 113 \pm 11$ kJ/mol, $\Delta S_H = 0.35 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (calculated-TSA, Burkhard 1984)
6.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.85 (recommended, Sangster 1993)
7.10 (estimated, Girvin & Scott 1997)
6.9132 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.67, 10.51; 10.64 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.38 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

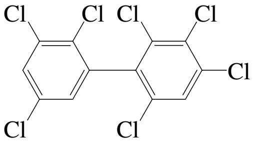
Biota Sediment Accumulation Factor, BSAF:
89 (trout in Lake Ontario, Niimi 1996)
0.29, 2.8, 1.4(grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K_{OC}:
6.94 (suspended particulate matter, Burkhard 1984)
5.52 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
5.82 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.60 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1979)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 160$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 194$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{1/2} = 160$ d for high-dose treatment, $t_{1/2} = 194$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.175 2,2′,3,3′,4,5′,6-Heptachlorobiphenyl (PCB-175)



Common Name: 2,2′,3,3′,4,5′,6-Heptachlorobiphenyl
Synonym: PCB-175, 2,2′,3,3′,4,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5′,6-heptachlorobiphenyl
CAS Registry No: 40186-70-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
  133 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.00557 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.00894 (20°C, supercooled liquid, Murphy et al. 1987)
  0.00104 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  4.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  7.00×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  7.72×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
  3.98×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
  $\log (P_L/\text{Pa}) = -4962/(T/\text{K}) + 12.22$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  49.55 (calculated-P/C, Burkhard 1984)
  22.63 (calculated-QSPR, Dunnivant et al. 1992)
  2.069 (calculated-QSPR, Achman et al. 1993)
  59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  7.19 (calculated-TSA, Burkhard 1984)
  6.92 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988a)
  7.17 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
  6.92 (recommended, Sangster 1993)
  7.10 (estimated, Girvin & Scott 1997)
  7.0957 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
  11.35, 10.17 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
  10.83 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:

144	(trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:

6.99	(suspended particulate matter, Burkhard 1984)
5.501	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.60	(soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

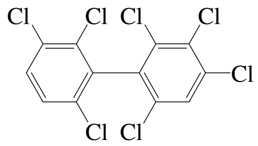
$k_2 = 0.005\ d^{-1}$ with $t_{½} = 154$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 169$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½} = 154$ d for high-dose treatment, $t_{½} = 169$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.176 2,2′,3,3′,4,6,6′-Heptachlorobiphenyl (PCB-176)



Common Name: 2,2′,3,3′,4,6,6′-Heptachlorobiphenyl
Synonym: PCB-176, 2,2′,3,3′,4,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,6,6′-heptachlorobiphenyl
CAS Registry No: 52663-65-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
101 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00601 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00585 (20°C, supercooled liquid, Murphy et al. 1987)
0.00280 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00314 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.66×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
5.31×10^{-4}, 8.83×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.35×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/mmHg) = 11.50 - 5080/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
4.17×10^{-4}, 7.24×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4579/(T/K) + 12.07$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
100 (calculated-P/C, Burkhard 1984)
9.12 (20°C, calculated-P/C, Murphy et al. 1987)
30.11 (calculated-QSPR, Dunnivant et al. 1992)
3.13 (calculated-QSPR, Achman et al. 1993)
107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.16 (calculated-TSA, Burkhard 1984)
6.55 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.76 (generator column-GC, Larsen et al. 1992)
6.65 (recommended, Sangster 1993)
6.6653 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.22, 10.06; 10.13 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.64 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.96 (suspended particulate matter, Burkhard 1984)
5.358 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

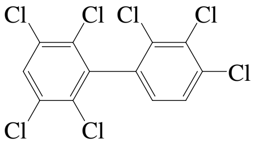
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004$ d^{-1} with $t_{½} = 184$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005$ d^{-1} with $t_{½} = 153$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½} = 184$ d for high-dose treatment, $t_{½} = 153$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.177 2,2′,3,3′,4,5′,6′-Heptachlorobiphenyl (PCB-177)



Common Name: 2,2′,3,3′,4,5′,6′-Heptachlorobiphenyl
Synonym: PCB-177, 2,2′,3,3′,4,5′,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5′,6′-heptachlorobiphenyl
CAS Registry No: 52663-70-4
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
145 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00656 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00482 (20°C, supercooled liquid, Murphy et al. 1987)
0.00150 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
4.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
4.40×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
4.88×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
2.50×10^{-4}, 3.38×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.15×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
1.38×10^{-4}, 2.51×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4962/(T/K) + 13.04$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
26.45 (calculated-P/C, Burkhard 1984)
3.34 (20°C, calculated-P/C, Murphy et al. 1987)
15.55 (calculated-QSPR, Dunnivant et al. 1992)
2.069 (calculated-QSPR, Achman et al. 1993)
5.12 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
50.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 112 \pm 11$ kJ/mol, $\Delta S_H = 0.34 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.12 (calculated-TSA, Burkhard 1984)
6.73 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.73 (recommended, Sangster 1993)

7.10 (estimated, Girvin & Scott 1997)
6.9207 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.74, 10.58 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

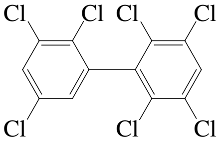
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.92 (suspended particulate matter, Burkhard 1984)
5.54, 5.39, 5.35, 4.90 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.359; 5.52 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, observed; calculated-molecular connectivity indices, Sabljic et al. 1989)
5.82 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.60 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.005\ d^{-1}$ with $t_{½} = 147$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 186$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½} = 147$ d for high-dose treatment, $t_{½} = 186$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.178 2,2′,3,3′,5,5′,6-Heptachlorobiphenyl (PCB-178)



Common Name: 2,2′,3,3′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-178, 2,2′,3,3′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-67-9
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):

125	(estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

330.9	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.00588	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00884	(20°C, supercooled liquid, Murphy et al. 1987)
0.001016	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.000627	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

6.57×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.24×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.47×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 11.70 - 5220/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
4.57×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4962/(T/K) + 13.28$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

44.08	(calculated-P/C, Burkhard 1984)
6.586	(20°C, calculated-P/C, Murphy et al. 1987)
2.33	(wetted wall column-GC/ECD, Brunner et al. 1990)
21.61	(calculated-QSPR, Dunnivant et al. 1992)
11.2	(11°C, gas stripping-GC/ECD, Bamford et al. 2002)
71.4	(from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 90 \pm 10$ kJ/mol, $\Delta S_H = 0.27 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.17	(calculated-TSA, Burkhard 1984)
6.85	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.14	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.85	(recommended, Sangster 1993)
7.0564	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.28, 10.12	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.33	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.97	(suspended particulate matter, Burkhard 1984)
5.501	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

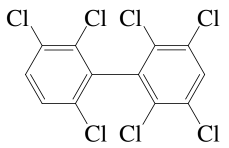
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½} = 156$ d for high-dose treatment, $t_{½} = 166$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.179 2,2′,3,3′,5,6,6′-Heptachlorobiphenyl (PCB-179)



Common Name: 2,2′,3,3′,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-179, 2,2′,3,3′,5,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,6,6′-heptachlorobiphenyl
CAS Registry No: 52663-64-6
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
 99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
 330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
 0.00632 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
 0.00454 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 0.0039 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 1.42×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
 1.55×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
 5.15×10^{-4}, 1.004×10^{-3} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 5.01×10^{-4}, 8.71×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/\text{Pa}) = -4579/(T/\text{K}) + 12.07$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
 88.96 (calculated-P/C, Burkhard 1984)
 2.432 (wetted wall column-GC/ECD, Brunner et al. 1990)
 27.91 (calculated-QSPR, Dunnivant et al. 1992)
 37.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 144 \pm 7$ kJ/mol, $\Delta S_H = 0.45 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
 6.77, 8.13 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
 7.14 (calculated-TSA, Burkhard 1984)
 6.41 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 6.73 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
 6.41 (recommended, Sangster 1993)
 6.6366 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.26, 10.10	(0, 20°C, multi-column k′ correlation, Zhang et al. 1999)
10.34	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.94	(suspended particulate matter, Burkhard 1984)
5.358	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 171$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 198$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

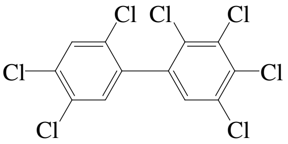
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 171$ d for high-dose treatment, $t_{1/2} = 198$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.180 2,2′,3,4,4′,5,5′-Heptachlorobiphenyl (PCB-180)



Common Name: 2,2′,3,4,4′,5,5′-Heptachlorobiphenyl
Synonym: PCB-180, 2,2′,3,4,4′,5,5′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,5′-heptachlorobiphenyl
CAS Registry No: 35065-29-3
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
 109–110 (Hutzinger et al. 1974)
Boiling Point (°C): 240–280 (20mm Hg)
Density (g/cm^3):
Molar Volume (cm^3/mol):
 330.9 (calculated-Le Bas method at normal boiling point)
 250.3 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
 56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
 0.144 (calculated-Mackay et al. 1992; Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
 0.00656 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
 0.00385 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
 0.00031 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 0.00063 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
 0.00053 (calculated-MCI χ, Patil 1991)
 2.45×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)
 log S_L (mol/L) = –1.676 + 1132/(T/K) (supercooled liquid, Passivirta et al. 1999)
 3.17×10^{-3}; 5.22×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)
 log S_L/(mol m^{-3}) = –1356/(T/K) – 0.33 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 8.10×10^{-5} (Verlag Chemie 1983)
 1.30×10^{-4}, 1.29×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
 8.07×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
 5.06×10^{-4} (supercooled liquid P_L, calculated-GC-RI correlation, Burkhard 1985b)
 1.21×10^{-4}, 1.43×10^{-4} (supercooled liquid. P_L, GC-RT correlation, different stationary phases Foreman & Bidleman 1985)
 3.14×10^{-5} (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
 8.13×10^{-5}, 1.20×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
 log (P_L/Pa) = – 5042/(T/K) + 13.03 (GC-RT correlation, Falconer & Bidleman 1994)
 1.45×10^{-4}, 2.09×10^{-5} (supercooled liquid P_L, solid P_S, Passivirta et al. 1999)
 log (P_S/Pa) = 15.98 – 6173/(T/K) (solid, Passivirta et al. 1999)
 log (P_L/Pa) = 13.03 – 5042/(T/K) (supercooled liquid, Passivirta et al. 1999)
 1.32×10^{-4}; 1.072×10^{-4} (supercooled P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 log P_L/Pa = –4809/(T/K) + 12.16 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

30.40 (calculated-P/C, Burkhard et al. 1985b)
3.24 (20°C, calculated-P/C, Murphy et al. 1987)
1.013 (wetted-wall column-GC/ECD, Brunner et al. 1990)
10.88 (calculated-QSPR, Dunnivant et al. 1992)
7.10 (estimated, Girvin & Scott 1997)
$\log H/(Pa\ m^3/mol) = 14.71 - 3910/(T/K)$ (Passivirta et al. 1999)
37.0* ± 0.20 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$K_{AW} = \exp[-(143.6/kJ{\cdot}mol^{-1})/\ RT] + (0.447/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where $R = 8.314\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
37.3 (exptl. data, Bamford et al. 2002)—see Comment by Goss et al. 2004
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 144 \pm 7$ kJ/mol, $\Delta S_H = 0.45 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
5.89, 8.51 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log H/(Pa\ m^3/mol) = -3453/(T/K) + 12.49$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.12 (calculated-TSA, Burkhard 1984)
6.70 (calculated-chlorine substituents, Oliver 1987a)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.36 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.02 (calculated-MCI χ, Patil 1991)
7.40 (calculated-TSA, Murray & Andren 1992)
6.56 (average, generator column-GC, Larsen et al. 1992)
6.89 (recommended, Sangster 1993)
7.2506 (calculated-molecular properties MNDO-AM1, Makino 1998)
7.20 (calculated, Passivirta et al. 1999)
7.29, 7.16 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

10.75* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
$\log K_{OA} = -4.70 + 4535/(T/K)$; (temp range –10 to 30°C, Harner & Bidleman 1996)
9.88; 9.72 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
$\log K_{OA} = -3.31 + 3930/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
11.22 (10°C, estimated, Thomas et al. 1998)
9.88 (quoted, Kömp & McLachlan 1997b; Kaupp & McLachlan 1999)
11.94, 10.72; 10.86 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.85 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
10.12, 10.16 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4975/(T/K) - 6.55$ (LDV linear regression of literature data, Li et al. 2003)
$\log K_{OA} = 4845/(T/K) - 6.09$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

2.99–5.68 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.22–6.41 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.45, 6.45 (*Daphnia magna*, 21-d exposure: wet wt basis, lipid wt basis, Geyer et al. 2000)
6.06, 7.36 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

6.92 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.2–7.4, 6.9; 7.30 (suspended sediments, range; average, algae > 50 µm, Oliver 1987a)
6.51 (Lake Michigan water column, Swackhamer & Armstrong 1987)

5.73, 5.54, 5.50, 5.09 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.73; 5.66 (marine humic substances at 5 mg/L DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
6.36, 6.23, 6.10 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.78 (Ispra soil, shake flask-GC/ECD, Paya-Perez et al. 1991)
6.60 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.60 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.53–7.76; 5.80–7.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.42; 6.56, 7.42, 6.83 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
6.31–6.98 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 0.049\ h^{-1}$; $k_1 = 0.008\ h^{-1}$ (mayfly-sediment model II, Gobas et al. 1989)
$k_2 = 0.0246\ d^{-1}$ with an elimination $t_{½}$ = 282 d (earthworm, Belfroid et al. 1995)
$k_1 = 0.00348\ h^{-1}$; $k_2 = 0.111\ h^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1(calc) = 2 (food lipid mg)/(g worm lipid-d); k_2(calc) = 0.03 d^{-1} (earthworm, Wågman et al. 2001)
$k_2 = 0.004\ d^{-1}$ with $t_{½}$ = 162 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½}$ = 186 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
$k_2 = 0.021\ d^{-1}$ with $t_{½}$ = 33.0 d (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:
Air: $t_{½}$ = 12000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: $t_{½}$ = 240000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: very persistent, $t_{½}$ = 25 yr (Geyer et al. 2000)
$t_{½}$ = 330000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{½}$ = 333000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: elimination $t_{½}$ = 28.3 d from earthworm (Belfroid et al. 1995);
elimination $t_{½}$ = 22 d in earthworm given contaminated food (predicted, Wågman et al. 2001)
depuration $t_{½}$ = 162 d for high-dose treatment, $t_{½}$ = 186 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
depuration $t_{½}$ = 33.0 d (juvenile carp in 100-d experiment Stapleton et al. 2004)

TABLE 7.1.1.180.1

Reported Henry's law constants and octanol-air partition coefficients of 2,2′,3,4,4′,5,5′-heptachlorobiphenyl (PCB-180) at various temperatures and temperature dependence equations

Henry's law constant		log K_{OA}	
Bamford et al. 2000		Harner & Bidleman 1996	
gas stripping-GC/MS		generator column-GC	
t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
4	0.425	–10	12.46
11	2.025	0	12.00
18	8.96	10	11.38
25	37.0	20	10.75
31	118.5	30	10.23
$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 86.83$	
A	53.7647		
B	17272	$\log K_{OA} = A + B/T$	
		A	–4.695
enthalpy, entropy change:		B	4535
$\Delta H/(\text{kJ·mol}^{-1}) = 143.6 \pm 7.4$			
$\Delta S/(\text{J·mol}^{-1}\text{·K}^{-1}) = 447 \pm 26$			

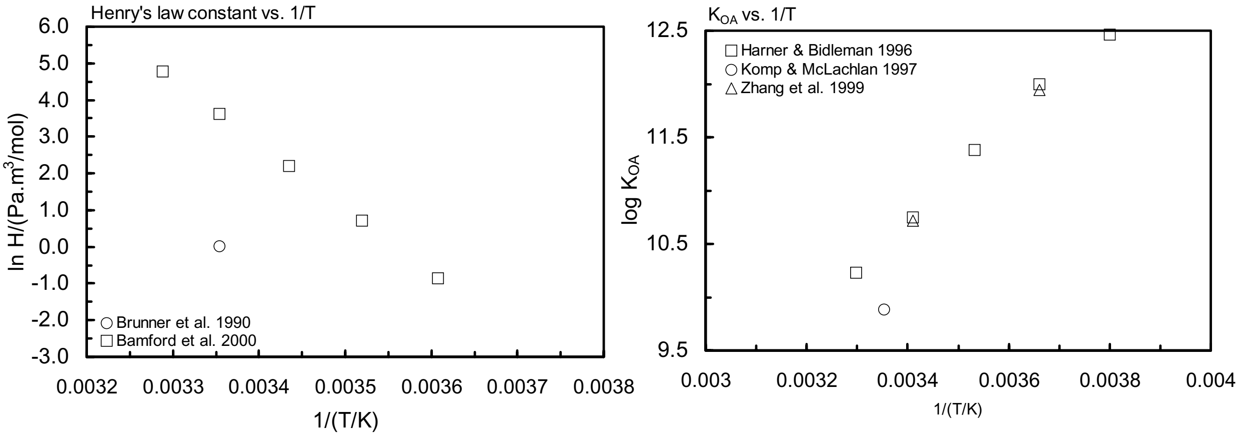
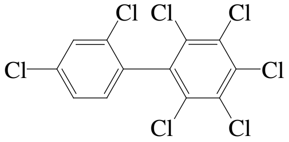


FIGURE 7.1.1.180.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,2′,3,4,4′,5,5′-heptachlorobiphenyl (PCB-180).

7.1.1.181 2,2′,3,4,4′,5,6-Heptachlorobiphenyl (PCB-181)



Common Name: 2,2′,3,4,4′,5,6-Heptachlorobiphenyl
Synonym: PCB-181, 2,2′,3,4,4′,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,6-heptachlorobiphenyl
CAS Registry No: 74472-47-2
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
140 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00625 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.44×10^{-4}, 5.21×10^{-4}; 2.30×10^{-4}, 4.54×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases Brodsky & Ballschmiter 1988)
3.95×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.44×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.11×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
2.92×10^{-4}, 4.206×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.54×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P_L/Pa) = -4962/(T/K) + 13.11$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
40.83 (calculated-P/C, Burkhard 1984)
23.31 (calculated-QSPR, Dunnivant et al. 1992)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (calculated-TSA, Burkhard 1984)
7.11, 7.12, 7.19, 7.11 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.13 (recommended, Sangster 1993)
7.0558 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.61 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log K_B or log BCF:

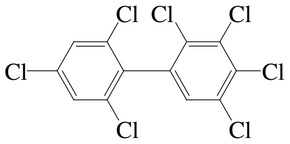
Sorption Partition Coefficient, log K_{OC}:

6.94	(suspended particulate matter, Burkhard 1984)
5.516	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

7.1.1.182 2,2′,3,4,4′,5,6′-Heptachlorobiphenyl (PCB-182)



Common Name: 2,2′,3,4,4′,5,6′-Heptachlorobiphenyl
Synonym: PCB-182, 2,2′,3,4,4′,5,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,6′-heptachlorobiphenyl
CAS Registry No: 60145-23-5
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
152 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0567 (mp at 152°C)

Water Solubility (g/m^3 or mg/L at 25°C):
5.34×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
8.26×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
3.95×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.36×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.31×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.43×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
3.66×10^{-4}, 3.56×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.14×10^{-4}, 3.72×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4962/(T/\text{K}) + 13.11$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
97.07 (calculated-P/C, Burkhard 1984)
26.04 (calculated-QSPR, Dunnivant et al. 1992)
2.07 (calculated-QSPR, Achman et al. 1993)
8.71 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
63.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 97 \pm 10$ kJ/mol, $\Delta S_H = 0.30 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.22 (calculated-TSA, Burkhard 1984)
6.92 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.92 (recommended, Sangster 1993)
7.0964 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

10.42	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.02	(suspended particulate matter, Burkhard 1984)
5.501	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calc-molecular connectivity indices, Sabljic et al. 1989)
6.10	(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 159$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 182$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

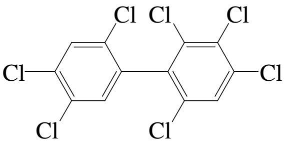
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½} = 159$ d for high-dose treatment, $t_{½} = 182$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.183 2,2′,3,4,4′,5′,6-Heptachlorobiphenyl (PCB-183)



Common Name: 2,2′,3,4,4′,5′,6-Heptachlorobiphenyl
Synonym: PCB-183, 2,2′,3,4,4′,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-69-1
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
  152 (estimated, Abramowitz & Yalkowsky 1990)
  83 (Kühne et al. 1995; Ruelle & Kesselring 1997; Ran et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  330.9 (calculated-Le Bas method at normal boiling point)
  250.3 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.270 (mp at 83°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.00534 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.00490 (20°C, supercooled liquid, Murphy et al. 1987)
  3.14×10^{-4}, 4.98×10^{-4}, 6.27×10^{-4}, 5.09×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  3.14×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
  0.000641 (calculated-group contribution method, Kühne et al. 1995)
  9.27×10^{-4}, 2.49×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
  1.77×10^{-3} (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  6.38×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  7.05×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
  3.57×10^{-4}, 5.09×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  8.61×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
  2.0×10^{-4}, 3.24×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
  $\log (P_L/\text{Pa}) = -4962/(T/\text{K}) + 13.19$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
  47.32 (calculated-P/C, Burkhard 1984)
  6.89 (20°C, calculated-P/C, Murphy et al. 1987)
  20.40 (calculated-QSPR, Dunnivant et al. 1992)
  2.069 (calculated-QSPR, Achman et al. 1993)
  0.326, 0.954 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
  8.02 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  61.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 100 \pm 10$ kJ/mol, $\Delta S_H = 0.30 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.22 (calculated-TSA, Burkhard 1984)
7.02, 7.13, 6.96, 7.07 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.78 (generator column-GC, Larsen et al. 1992)
6.92 (recommended, Sangster 1993)
7.0868 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
8.27 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.80 (10°C, estimated, Thomas et al. 1998)
11.44, 10.26; 10.35 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.83 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.84, 7.37 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor, BSAF:

220 (trout in Lake Ontario, Niimi 1996)
0.52, 4.2, 0.84 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K_{OC}:

7.02 (suspended particulate matter, Burkhard 1984)
5.53, 5.40, 5.35, 4.92 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.53; 5.50 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, observed; calculated-molecular connectivity indices, Sabljic et al. 1989)
6.36, 6.25, 6.09 (North Sea sediments, field measurement-GC/ECD, Lara & Ernst 1990)
5.82 (Ispra soil, batch equilibrium-GC/ECD, Paya-Perez et al. 1991)

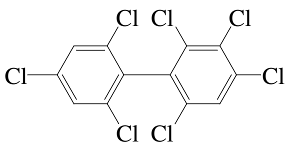
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 165$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003\ d^{-1}$ with $t_{½} = 206$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 165 d for high-dose treatment, $t_{½}$ = 206 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.184 2,2′,3,4,4′,6,6′-Heptachlorobiphenyl (PCB-184)



Common Name: 2,2′,3,4,4′,6,6′-Heptachlorobiphenyl
Synonym: PCB-184, 2,2′,3,4,4′,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,6,6′-heptachlorobiphenyl
CAS Registry No: 74472-48-3
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
108 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00514 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00198 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.65×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.80×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
126.7 (calculated-P/C, Burkhard 1984)
46.42 (calculated-QSPR, Dunnivant et al. 1992)
3.94 (calculated-QSPR, Achman et al. 1993)
107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.23 (calculated-TSA, Burkhard 1984)
6.85 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.76 (generator column-GC, Larsen et al. 1992)
6.65 (recommended, Sangster 1993)
6.8203 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.73 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
7.03 (suspended particulate matter, Burkhard 1984)
5.342 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

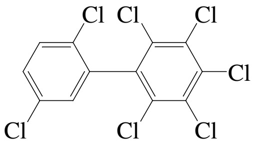
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 2 (food lipid mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 20 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.185 2,2′,3,4,5,5′,6-Heptachlorobiphenyl (PCB-185)



Common Name: 2,2′,3,4,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-185, 2,2,3,4,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52712-05-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
149 (Bruggeman et al. 1982; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3702
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0607 (mp at 149°C)
0.0595 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00047 (generator column-GC/ECD, Weil et al. 1974)
0.00546 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
5.71×10^{-4}, 8.26×10^{-4}, 6.27×10^{-4}, 6.56×10^{-4} (RP- HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.75×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
7.28×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.21×10^{-4}, 4.78×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.70×10^{-4}, 2.95×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4962/(T/K) + 13.15$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
46.0 (calculated-P/C, Burkhard et al. 1985b)
1.62 (wetted-wall column-GC, Brunner et al. 1990)
21.71 (calculated-QSPR, Dunnivant et al. 1992)
2.67 (calculated-QSPR, Achman et al. 1993)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.93 (TLC-RT correlation, Bruggeman et al. 1982)
7.01, 6.98, 6.96, 7.00 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.99 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

10.58	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.36	(*Picea omorika*, Reischl et al. 1989 from Reischl 1988)
5.93; 7.46	(22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.93, 7.47	(zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.95	(Koch 1983)
6.94	(suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.52	(marine humic substances of 5 mg/L DOC, calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
5.33	(calculated-K_{OW}, Bahnick & Doucette 1988)
6.43	(calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.28	(calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
6.29. 6.08, 6.13	(North Sea sediments, field measurement-GC/ECD, Lara & Ernst 1990)
5.80	(calculated-MCI, Park & Lee 1993)
6.50	(soil, calculated-K_{OW}, Girvin & Scott 1997)
6.40	(soil, calculated-universal solvation model; Winglet et al. 2000)

Sorption Partition Coefficient, log K_{OM}:

5.95, 5.31	(selected, calculated-molecular connectivity indices χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 5810 d^{-1}; k_2 = 0.00677 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.004 d^{-1} with $t_{½}$ = 156 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

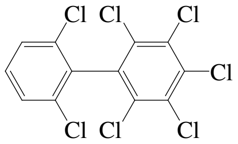
k_2 = 0.004 d^{-1} with $t_{½}$ = 184 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 48 d in *Picea omorika* (Reischl et al. 1989 from Reischl 1988).

depuration $t_{½}$ = 156 d for high-dose treatment, $t_{½}$ = 184 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.186 2,2′,3,4,5,6,6′-Heptachlorobiphenyl (PCB-186)



Common Name: 2,2′,3,4,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-186
Chemical Name: 2,2′,3,4,5,6,6′-heptachlorobiphenyl
CAS Registry No: 74472-49-4
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
    142 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
    330.9 (Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
    0.00672 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
    0.00157 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    1.35×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
    1.47×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
    4.68×10^{-4}, 7.55×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
    $\log (P_L/\text{Pa}) = -4579/(T/K) + 12.03$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
    79.13 (calculated-P/C, Burkhard 1984)
    37.3 (calculated-QSPR, Dunnivant et al. 1992)
    107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
    $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
    7.11 (calculated-TSA, Burkhard 1984)
    6.69 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
    6.7069 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
    10.36 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
    6.91 (suspended particulate matter, Burkhard 1984)
    5.383 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

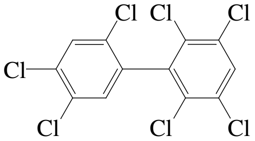
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota:

7.1.1.187 2,2′,3,4′,5,5′,6-Heptachlorobiphenyl (PCB-187)



Common Name: 2,2′,3,4′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-187, 2,2′,3,4′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-68-0
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
  149.0 (Mackay et al. 1980; Burkhard et al. 1985a)
  147 (Ruelle & Kesselring 1997)
Boiling Point (°C):
  417 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm^3):
Molar Volume (cm^3/mol):
  330.9 (calculated-Le Bas method at normal boiling point)
  250.3 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0607 (mp at 149°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  4.70×10^{-4} (generator column-GC/ECD, Weil et al. 1974)
  0.00451 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  0.0826 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  3.05×10^{-4} (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
  3.92×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
  5.98×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
  3.47×10^{-4}, 5.74×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  9.42×10^{-5} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  2.14×10^{-4}, 3.72×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
  $\log (P_L/\text{Pa}) = -4977/(T/K) + 12.96$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
  42.15 (calculated-P/C, Burkhard et al. 1985b)
  8.41 (20°C, calculated-P/C, Murphy et al. 1987)
  20.55 (calculated-QSPR, Dunnivant et al. 1992)
  2.07 (calculated-QSPR, Achman et al. 1993)
  3.304, 8.72, 23.84, 82.20 ± 2.2, 136.7 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
  $\ln K_{AW} = 35.242 - 11582.87/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
  $K_{AW} = \exp[-(96.3/\text{kJ·mol}^{-1})/RT] + (0.293/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
  65.9 (exptl. data, Bamford et al. 2002)
  $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 96 ± 7 kJ/mol, ΔS_H = 0.29 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.19 (calculated-TSA, Burkhard 1984)
6.92 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
7.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.40 (calculated-TSA, Murray & Andren 1992)
6.76 (generator column-GC, Larsen et al. 1992)
6.84 (recommended, Sangster 1993)
7.10 (estimated, Girvin & Scott 1997)
7.0464 (calculated-molar properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

9.87; 9.25 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log $K_{OA} = -5.20 + 4490/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
10.85 (10°C, estimated, Thomas et al. 1998)
11.36, 10.22 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.54 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.51–5.48 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.94–6.05 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Biota Sediment Accumulation Factor, BSAF:

244 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:

6.99 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.51, 5.40, 5.33, 4.90 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.51; 5.50 (marine humic substances of 5 mg/L DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
6.60 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.60 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.40; 6.00 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

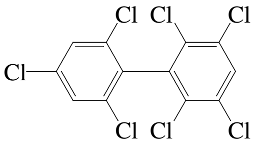
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.005\ d^{-1}$ with $t_{1/2} = 131$ d and $k_2 = 0.010\ d^{-1}$ with $t_{1/2} = 71$ d for food concn of 22 ng/g and 125 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 159$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 190$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{1/2}$ = 71–131 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{1/2}$ = 159 d for high-dose treatment, $t_{1/2}$ = 190 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.188 2,2′,3,4′,5,6,6′-Heptachlorobiphenyl (PCB-188)



Common Name: 2,2′,3,4′,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-188, 2,2′,3,4′,5,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,6,6′-heptachlorobiphenyl
CAS Registry No: 74487-85-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
130 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00538 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00451 (20°C, supercooled liquid, Murphy et al. 1987)
0.00128 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00125 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.55×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55×10^{-4}, 1.69×10^{-3}, 2.96×10^{-5} (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
8.51×10^{-4}, 1.50×10^{-3} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.42×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P_L/\text{Pa}) = -4579/(T/\text{K}) + 13.29$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
113.5 (calculated-P/C, Burkhard 1984)
8.41 (20°C, calculated-P/C, Murphy et al. 1987)
44.95 (calculated-QSPR, Dunnivant et al. 1992)
15.77, 31.39, 60.5, 113.1 ± 4.0, 188.6 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 21.891 - 7457.3/(T/\text{K})$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(62.0/\text{kJ·mol}^{-1})/RT] + (0.182/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
107.9 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.21 (calculated-TSA, Burkhard 1984)
6.78 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

6.82	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.78	(recommended, Sangster 1993)
6.7947	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

10.22	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.01	(suspended particulate matter, Burkhard 1984)
5.342	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

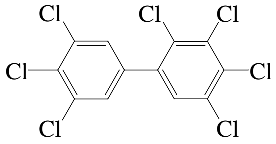
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 2 (food lipid mg)/(g worm lipid-d); $k_{2:}$ = 0.03 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 21 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.189 2,3,3′,4,4′,5,5′-Heptachlorobiphenyl (PCB-189)



Common Name: 2,3,3′,4,4′,5,5′-Heptachlorobiphenyl
Synonym: PCB-189, 2,3,3′,4,4′,5,5′-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5,5′-heptachlorobiphenyl
CAS Registry No: 39635-31-9
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
170 (Burkhard et al. 1985b)
163 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0378 (mp at 170°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0063 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
7.53×10^{-5} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.26×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.30×10^{-4}; 4.47×10^{-5} (generator column-GC/ECD, estimated, Hong & Qiao 1995)
4.05×10^{-4} (calculated-mp and K_{OW}, Ran et al. 2002)
0.000063 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000029, 0.000044, 0.000063, 0.000136 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.44×10^{-4} (P_L supercooled liquid GC-RT correlation, Burkhard et al. 1985a)
5.95×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
4.77×10^{-5}, 3.30×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.69×10^{-5} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -5300/(T/K) + 13.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
9.18 (calculated-P/C, Burkhard et al. 1985a)
6.74 (calculated-QSPR, Dunnivant et al. 1992)
0.903 (calculated-QSPR, Achman et al. 1993)
28.8 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (calculated-TSA, Burkhard 1984)
7.72 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.75 (generator column-GC, Larsen et al. 1992)
7.24 (recommended, Sangster 1993)
7.15 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.81, 11.54; 11.45 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.15 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

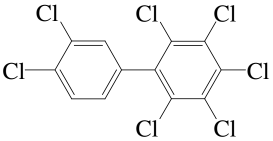
Bioconcentration Factor, log BCF or log K_B:
6.41, 7.71 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
6.94 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.817 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.011\ d^{-1}$ with $t_{1/2} = 64$ d and $k_2 = 0.012\ d^{-1}$ with $t_{1/2} = 58$ d for food concn of 19 ng/g and 138 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 176$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 171$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: reported biological $t_{1/2} > 200$ d for heptachlorobiphenyls in carp (Niimi 1987)
Depuration $t_{1/2} = 58$–64 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{1/2} = 176$ d for high-dose treatment, $t_{1/2} = 171$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.190 2,3,3′,4,4′,5,6-Heptachlorobiphenyl (PCB-190)



Common Name: 2,3,3′,4,4′,5,6-Heptachlorobiphenyl
Synonym: PCB-190, 2,3,3′,4,4′,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5,6-heptachlorobiphenyl
CAS Registry No: 41411-64-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):

117.0	(Burkhard et al. 1985b)
116	(Brodsky & Ballschmiter 1988)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):

330.9	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.125 (mp at 117°C)

Water Solubility (g/m^3 or mg/L at 25°C):

0.00767	(S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.98×10^{-4}	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.98×10^{-4}	(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
2.20×10^{-4}	(calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

1.96×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.70×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
1.09×10^{-4}, 1.47×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.13×10^{-5}, 7.08×10^{-5} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5109/(T/K) + 13.17$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

10.06	(calculated-P/C, Burkhard 1984)
11.37	(calculated-QSPR, Dunnivant et al. 1992)
28.8	(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.05	(calculated-TSA, Burkhard 1984)
7.08	(RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.46	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.08	(recommended, Sangster 1993)
7.2887	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.09, 10.87	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.90	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.84 (suspended particulate matter, Burkhard 1984)
5.675 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

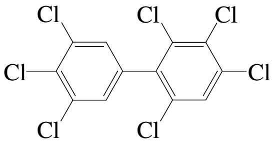
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 2 (food lipid (mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{½}$ = 160 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 184 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 25 d in earthworm given contaminated food (Wågman et al. 2001)
depuration $t_{½}$ = 160 d for high-dose treatment, $t_{½}$ = 184 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.191 2,3,3′,4,4′,5′,6-Heptachlorobiphenyl (PCB-191)



Common Name: 2,3,3′,4,4′,5′,6-Heptachlorobiphenyl
Synonym: PCB-191, 2,3,3′,4,4′,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5′,6-heptachlorobiphenyl
CAS Registry No: 74472-50-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
126 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
6.60×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.14×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.89×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55×10^{-4}, 2.04×10^{-4}, 5.68×10^{-6} (supercooled liquid P_L, calculated- MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.05×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -5109/(T/K) + 13.15$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
17.33 (calculated-P/C, Burkhard 1984)
13.48 (calculated-QSAR, Dunnivant et al. 1992)
1.367 (calculated-QSPR, Achman et al. 1993)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.12 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.55 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.3254 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.07, 10.91; 10.93 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.10 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

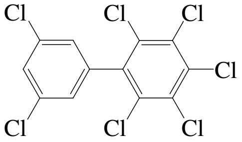
Sorption Partition Coefficient, log K_{OC}:

6.92	(suspended particulate matter, Burkhard 1984)
5.659	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

7.1.1.192 2,3,3′,4,5,5′,6-Heptachlorobiphenyl (PCB-192)



Common Name: 2,3,3′,4,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-192, 2,3,3′,4,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5,5′,6-heptachlorobiphenyl
CAS Registry No: 74472-51-8
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
142 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
6.92×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.14×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.57×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.89×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55×10^{-4}, 3.23×10^{-4}, 2.96×10^{-5} (P_L, calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.75×10^{-4}, 2.49×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.12×10^{-5}, 1.41×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5109/(T/K) + 13.38$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
16.52 (calculated-P/C, Burkhard 1984)
19.40 (calculated-QSPR, Dunnivant et al. 1992)
1.37 (calculated-QSPR, Achman et al. 1993)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.09 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.52 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.409 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

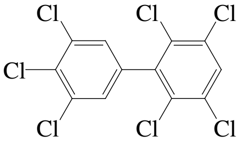
Sorption Partition Coefficient, log K_{OC}:

6.89	(suspended particulate matter, Burkhard 1984)
5.659	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

7.1.1.193 2,3,3′,4′,5,5′,6-Heptachlorobiphenyl (PCB-193)



Common Name: 2,3,3′,4′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-193, 2,3,3′,4′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 69782-91-8
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
154 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
6.96×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.14×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.25×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.70×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.91×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.37×10^{-4}, 8.79×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
7.59×10^{-5}, 1.20×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5109/(T/K) + 13.27$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
9.70 (calculated-P/C, Burkhard 1984)
13.61 (calculated-QSPR, Dunnivant et al. 1992)
1.37 (calculated-QSPR, Achman et al. 1993)
1.93 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 140 \pm 13$ kJ/mol, $\Delta S_H = 0.43 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.09 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.52 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.409 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.99, 10.82; 10.02 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)	
10.93	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.89	(suspended particulate matter, Burkhard 1984)
5.659	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 5 (food lipid mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air:

Surface water:

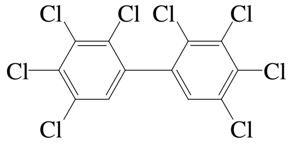
Ground water:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 21 d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.194 2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl (PCB-194)



Common Name: 2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl
Synonym: PCB-194, 2,2′,3,3′,4,4′,5,5′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,5′-octachlorobiphenyl
CAS Registry No: 35694-08-7
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
159–160 (Binns & Suschitzky 1971)
156 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3): 1.507 (at 22°C)
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
263.2 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0484 (mp at 159°C)
0.0474 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0072 (shake flask-GC/ECD, Wallnöfer et al. 1973)
0.000272 (generator column-GC/ECD, Weil et al. 1974)
8.58×10^{-5} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00124 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
3.79×10^{-3}; 2.40×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -1533/(T/K) - 0.11$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.03×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
3.86×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
2.07×10^{-5}, 1.79×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.29×10^{-5} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -5402/(T/K) + 13.43$ (GC-RT correlation, Falconer & Bidleman 1994)
2.04×10^{-5}; 2.45×10^{-5} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/Pa = -5099/(T/K) + 12.49$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
47.52 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
10.13 (wetted-wall column-GC, Brunner et al. 1990)
6.79 (calculated-QSPR, Dunnivant et al. 1992)
1.01 (calculated-QSPR, Achman et al. 1993)
0.34 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
10.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 169 \pm 6$ kJ/mol, $\Delta S_H = 0.52 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
6.76, 4.37 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(\text{Pa m}^3/\text{mol})] = -3566/(T/K) + 12.60$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
8.68 (RP-TLC-RT correlation, Bruggeman et al. 1982)
9.35 (HPLC-RT correlation, Shaw & Connell 1982)
7.62 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.67 (generator column-GC, Hawker & Connell 1988a)
6.94 (generator column-GC, Larsen et al. 1992)
7.65 (recommended, Sangster 1993)
7.67, 7.80, 9.35 (quoted lit. values, Hansch et al. 1995)
7.67, 7.76 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
10.50 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
12.83, 11.59; 11.71 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.17 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
11.31, 11.13 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4906/(T/K) - 5.33$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:
5.81 (guppy, 3.5% lipid, Bruggeman et al. 1984; quoted, Gobas et al. 1987)
4.35 (guppy, Gobas et al. 1987; quoted, Banerjee & Baughman 1991)
4.18 (worms, Oliver 1987c)
4.35 (guppy, calculated-C_B/C_W, or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
4.81 (guppy, estimated, Banerjee & Baughman 1991)
5.81; 7.34 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.81, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

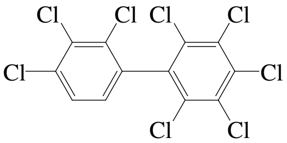
Sorption Partition Coefficient, log K_{OC}:
7.27 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.5–7.1, 6.8; 7.80 (suspended sediment, average; algae > 50 μm, Oliver 1987a)
5.94, 5.72, 5.68, 5.36 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.943, 6.016 (marine humic substances or 5 mg/L DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
6.41, 6.20, 6.06 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
6.96 (soil, calculated-Characteristic Root Index CRI model, Saçan & Balcioğlu 1996)
7.30 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 150$ d^{-1}; $k_2 = 0.007$ d^{-1} (guppy, Bruggeman et al. 1984)
$k_1 = 1000$ d^{-1} (guppy, Opperhuizen 1986)

log k_1 = 2.18 d^{-1}; log $1/k_2$ = 2.15 d (fish, quoted, Connell & Hawker 1988)
k_1 = 5640 d^{-1}; k_2 = 0.00865 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{½}$ = 158 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 174 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ > 1000 d in rainbow trout and $t_{½}$ = 78 d in its muscle (Niimi & Oliver 1983);
$t_{½}$ = 100 d in guppy (Bruggeman et al. 1984);
$t_{½}$ = 220 d in worms at 8°C (Oliver 1987c).
depuration $t_{½}$ = 158 d for high-dose treatment, $t_{½}$ = 174 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.195 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl (PCB-195)



Common Name: 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl
Synonym: PCB-195, 2,2′,3,3′,4,4′,5,6-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl
CAS Registry No: 52663-78-2
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
 176 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
 351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
 0.00334 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
 2.204×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
 9.92×10^{-5} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
 1.12×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
 4.53×10^{-5}, 7.46×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 2.19×10^{-5}, 3.63×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/\text{Pa}) = -5244/(T/\text{K}) + 13.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
 12.77 (calculated-P/C, Burkhard 1984)
 1.115 (wetted-wall column-GC/ECD, Brunner et al. 1990)
 12.01 (calculated-QSPR, Dunnivant et al. 1992)
 14.13 ± 0.78 (gas stripping-GC/ECD, measured range 4–31°C, Bamford et al. 2000)
 0.079, 0.485, 2.724, 14.13, 54.5 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
 $\ln K_{AW} = 62.305 - 20086.6/(T/\text{K})$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(167.0/\text{kJ·mol}^{-1})/\ RT] + (0.518/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
 15.1 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 167 ± 13 kJ/mol, ΔS_H = 0.52 ± 0.05 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
 7.49 (calculated-TSA, Burkhard 1984)
 7.35 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
 7.56 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.95 (generator column-GC, Larsen et al. 1992)
7.15 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.13, 10.04; 10.02 (0, 20°C, GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.26 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

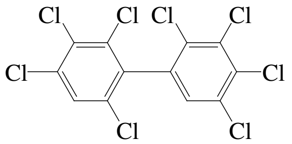
Bioconcentration Factor, log BCF or log K_B:
5.92; 7.45 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:
7.29 (suspended particulate matter, Burkhard 1984)
5.78, 5.59, 5.55, 5.32 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.78; 5.87 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
6.42, 6.26, 6.14 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 = 5930\ d^{-1}$; $k_2 = 0.00711\ d^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.010\ d^{-1}$ with $t_{1/2} = 67$ d and $k_2 = 0.011\ d^{-1}$ with $t_{1/2} = 61$ d for food concn of 24 ng/g and 126 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.005\ d^{-1}$ with $t_{1/2} = 143$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 158$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{1/2} = 61–67$ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{1/2} = 143$ d for high-dose treatment, $t_{1/2} = 158$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.196 2,2′,3,3′,4,4′,5,6′-Octachlorobiphenyl (PCB-196)



Common Name: 2,2′,3,3′,4,4′,5,6′-Octachlorobiphenyl
Synonym: PCB-196, 2,2′,3,3′,4,4′,5,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,6′-Octachlorobiphenyl
CAS Registry No: 42740-50-1
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
2.91×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.63×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.87×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.40×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
6.11×10^{-5}, 8.41×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.47×10^{-5}, 5.89×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5244/(T/\text{K}) + 13.37$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
71.94 (calculated-P/C, Burkhard 1984)
1.013 (wetted wall column-GC/ECD, Brunner et al. 1990)
13.23 (calculated-QSPR, Dunnivant et al. 1992)
0.990 (calculated-QSPR, Achman et al. 1993)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.57 (calculated-TSA, Burkhard 1984)
7.43 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.65 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.43 (recommended, Sangster 1993)
7.70 (estimated, Girvin & Scott 1997)
7.4190 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.27, 11.03; 11.19 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.40 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.37 (suspended particulate matter, Burkhard 1984)
5.857 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
7.30 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

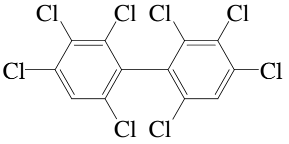
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 168$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½} = 156$ d for high-dose treatment, $t_{½} = 168$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.197 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl (PCB-197)



Common Name: 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl
Synonym: PCB-197, 2,2′,3,3′,4,4′,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl
CAS Registry No: 33091-17-7
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
132 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0892 (mp at 132°C)

Water Solubility (g/m^3 or mg/L at 25°C):
2.81×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.41×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.71×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.03×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6.79×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.93×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
1.90×10^{-4}, 1.22×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.12×10^{-5} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4581/(T/\text{K}) + 12.52$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
94.03 (calculated-P/C, Burkhard 1984)
25.69 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.59 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.30 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.74, 10.52; 10.68 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.30 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

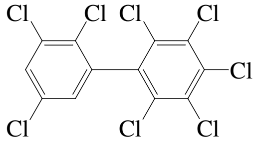
Sorption Partition Coefficient, log K_{OC}:

7.39	(suspended particulate matter, Burkhard 1984)
5.699	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.198 2,2′,3,3′,4,5,5′,6-Octachlorobiphenyl (PCB-198)



Common Name: 2,2′,3,3′,4,5,5′,6-Octachlorobiphenyl
Synonym: PCB-198, 2,2′,3,3′,4,5,5′,6-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′,6-Octachlorobiphenyl
CAS Registry No: 68194-17-2
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
162 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
3.03×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.63×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
8.58×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
1.48×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.44×10^{-4}, 1.67×10^{-4}, 5.68×10^{-6} (GC-RI correlation, Burkhard et al. 1985b)
6.85×10^{-5}, 1.224×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.01×10^{-5}, 7.08×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5244/(T/K) + 13.42$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
20.97 (calculated-P/C, Burkhard 1984)
1.419 (wetted wall column-GC/ECD, Brunner et al. 1990)
15.62 (calculated-QSPR, Dunnivant et al. 1992)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.55 (calculated-TSA, Burkhard 1984)
7.43 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.62 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.43 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.32, 11.05; 10.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.35 (suspended particulate matter, Burkhard 1984)

5.91, 5.63, 5.56, 5.23 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)

5.91; 5.86 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 158$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{1/2} = 185$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

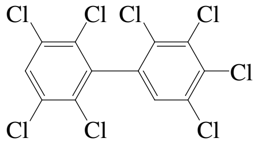
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 158$ d for high-dose treatment, $t_{1/2} = 185$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.199 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl (PCB-199)



Common Name: 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl
Synonym: PCB-199, 2,2′,3,3′,4,5,5′,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl
CAS Registry No: 52663-75-9
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
3.23×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.41×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.41×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.20×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.57×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
9.35×10^{-5}, 1.67×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.05×10^{-4}, 2.04×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, reported as the revised order PCB-200-2,2′,3,3′,4,5,6,6′- Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5244/(T/K) + 13.36$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
42.66 (calculated-P/C, Burkhard 1984)
1.013 (wetted wall column-GC/ECD, Brunner et al. 1990)
23.0 (calculated-QSPR, Dunnivant et al. 1992)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.51 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.28 (quoted lit., Maruya & Lee 1998-reported as revised order PCB-200: 2,2′,3,3′,4,5,6,6′-PCB)
7.21 (revised previously quoted value; Maruya & Lee 2000)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.28, 11.05; 10.02 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:

96 (trout in Lake Ontario, Niimi 1996)
0.26, 7.1, 1.1(grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

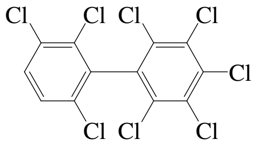
Sorption Partition Coefficient, log K_{OC}:

7.31 (suspended particulate matter, Burkhard 1984)
5.94, 5.72, 5.68, 5.36 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.711 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.44, 6.18, 6.02 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

7.1.1.200 2,2′,3,3′,4,5,6,6′-Octachlorobiphenyl (PCB-200)



Common Name: 2,2′,3,3′,4,5,6,6′-Octachlorobiphenyl
Synonym: PCB-200, 2,2′,3,3′,4′,5,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,6,6′-Octachlorobiphenyl
CAS Registry No: 52663-73-7
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
130 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
2.93×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.105×10^{-4}, 1.79×10^{-4}, 1.08×10^{-4}, 2.01×10^{-4} (RP-HPLC-k′ correlation, different and mobile stationary phases, Brodsky & Ballschmiter 1988)
4.30×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.56×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
6.37×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.75×10^{-4}, 3.32×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.89×10^{-5}, 5.89×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, reported in revised order as PCB-201-2,2′,3,3′,4,5′,6,6′-, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4851/(T/K) + 12.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
2.34×10^{-5} (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry’s Law Constant (Pa·m^3/mol at 25°C):
66.98 (calculated-P/C, Burkhard 1984)
1.50 (calculated-QSPR, Achman et al. 1993)
24.36 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.57 (calculated-TSA, Burkhard 1984)
7.16, 7.54, 7.16, 7.36; 7.35 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.35 (recommended, Sangster 1993)
7.27 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

8.16; 7.27–7.30 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
7.63; 7.28 (previously quoted; revised value, Maruya & Lee 2000)
7.32 (calculated-QSPR, Yeh & Hong 2002- reported as PCB-201 for 2,2′,3,3′,4,5,6,6′-octachlorobiphenyl)

Octanol/Air Partition Coefficient, log K_{OA} at 25°Cor as indicated:
12.05, 10.82 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

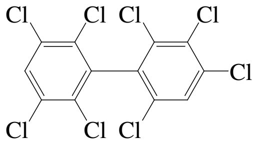
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
7.36 (suspended particulate matter, Burkhard 1984)
5.50, 5.72, 5.68, 5.36 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.68; 5.70 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
7.05 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.201 2,2′,3,3′,4,5′,6,6′-Octachlorobiphenyl (PCB-201)



Common Name: 2,2′,3,3′,4,5′,6,6′-Octachlorobiphenyl
Synonym: PCB-201, 2,2′,3,3′,4,5,5′,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3′,3′,4,5′,6,6′-Octachlorobiphenyl
CAS Registry No: 40186-71-8
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
162 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
3.06×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
2.204×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
8.58×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.56×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.06×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
5.94×10^{-5}, 1.0×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.41×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, reported as revised order PCB-199, 2,2′,3,3′,4,5,5′,6′-octachlorobiphenyl, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4581/(T/\text{K}) + 12.51$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
64.54 (calculated-P/C, Burkhard 1984)
1.72 (wetted wall column-GC/ECD, Brunner et al. 1990)
13.23 (calculated-QSPR, Dunnivant et al. 1992)
0.990 (calculated-QSPR, Achman et al. 1993)
0.156, 0.457 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
95.8 ± 4.4 (gas stripping-GC/ECD, measured range 4–31°C, Bamford et al. 2000)
1.069, 5.14, 22.98, 95.8, 308 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(144.5/\text{kJ·mol}^{-1})/RT] + (0.458/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
97.5 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 145 ± 7 kJ/mol, ΔS_H = 0.46 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.54 (calculated-TSA, Burkhard 1984)
7.35 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

7.21 (generator column-GC, Hawker & Connell 1988)
7.62 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.80 (calculated-TSA, Murray & Andren 1992)
7.31 (recommended, Sangster 1993)
7.70 (estimated, Girvin & Scott 1997)
7.21 (quoted lit., Maruya & Lee 1998, reported as the revised order PCB-199, 2,2′,3,3′,4′,5,5′,6-octachlorobiphenyl)
7.62 (revised previously quoted value, Maruya & Lee 2000)
7.21; 7.32 (quoted exptl.-generator column method; calculated-QSPR, Yeh & Hong 2002, reported as PCB-201 for 2,2′3,3′,4,5,6,6′-octachlorobiphenyl-should be PCB-200 in B&Z/IUPAC numbering system for 2,2′,3,3′,4,5,5′,6-octachlorobiphenyl)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.22, 10.98 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.30 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

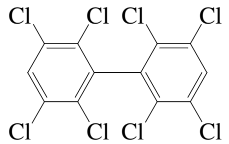
Bioconcentration Factor, log BCF or log K_B:
5.88; 7.41 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:
7.34 (suspended particulate matter, Burkhard 1984)
5.913; 5.857 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
6.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
7.30 (soil, estimated-log K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 = 5950\ d^{-1}$; $k_2 = 0.00776\ d^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.005\ d^{-1}$ with $t_{½} = 153$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 172$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½} = 153$ d for high-dose treatment, $t_{½} = 172$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.202 2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl (PCB-202)



Common Name: 2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl
Synonym: PCB-202, 2,2′,3,3′,5,5′,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl
CAS Registry No: 2136-99-4
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
161 (Van Roosmalen 1934; Burkhard et al. 1985a; Erickson 1986; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.507
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
263.2 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22.80 (Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
52.72 (Miller et al. 1984; Shiu & Mackay 1986; selected, Hinckley et al. 1990)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0463 (mp at 161°C)
0.0443 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.80×10^{-4} (generator column-GC/ECD, Weil et al. 1974;)
3.93×10^{-4} (generator column-GC/ECD, Miller et al. 1984,1985)
1.47×10^{-4}* (generator column-GC/ECD, measured range 20–50°C, Dickhut et al. 1986)
1.14×10^{-4}, 1.47×10^{-4}, 2.12×10^{-4}, 4.66×10^{-4} (4. 20, 25, 32°C, generator column-GC/ECD, Dickhut et al. 1986)
$\ln x = -6098/(T/K) - 5.333$, temp range 4–32°C, ΔH_{ss} = 50.7 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
$\log x = -2652/(T/K) - 2.308$, ΔH_{ss} = 50.6 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
$S/(mol/L) = 6.91 \times 10^{-11} \exp(0.064 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
2.53×10^{-4}, 5.93×10^{-4}, 6.51×10^{-4}, 2.36×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
$\ln x = -5.34 - 6100/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.90×10^{-5}* (extrapolated gas saturation-GC, measured range 29–61.2°C, Burkhard et al. 1984)
$\log (P/Pa) = 13.262 - 5307.3/(T/K)$; temp range 29–61.2°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)
2.89×10^{-5}, 6.43×10^{-4} (solid P_S, P_L calculated from P_S using fugacity ratio F, Burkhard et al. 1985a)
5.40×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
1.70×10^{-4}, 3.91×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
6.59×10^{-4}, 5.26×10^{-4} (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
2.22×10^{-4} (P_{GC} by GC-RT correlation with *p,p′*-DDT as reference standard, Hinckley et al. 1990)

log P_L/Pa = 12.99 – 4851/(T/K) (GC-RT correlation, Hinckley et al. 1990)
2.40×10^{-4} (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 4851/(T/K) + 12.99 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
$(2.41 - 29.5) \times 10^{-6}$; $(1.73 - 5.40) \times 10^{-4}$ (literature solid P_S range; literature liquid P_L range, Delle Site 1997)
log (P/Pa) = 13.282 – 5307.3/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C):
75.79 (calculated-P/C, Burkhard et al. 1985b)
38.08 (calculated-P/C, Shiu & Mackay 1986)
1.82 (wetted-wall column-GC, Brunner et al. 1990)
22.63 (calculated-QSPR, Dunnivant et al. 1992)
1.50 (calculated-QSPR, Achman et al. 1993)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 145 ± 7 kJ/mol, ΔS_H = 0.46 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
9.77 (Hansch & Leo 1979)
8.42 (TLC-RT correlation, Bruggeman et al. 1982)
7.11 (generator column-GC/ECD, Miller et al. 1984, 1985)
7.14 (generator column-HPLC, Woodburn et al. 1984)
7.12 (generator column-GC/ECD, Doucette & Andren 1987,1988)
7.01, 7.35, 6.98, 7.31 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.21 (generator column-GC, Hawker & Connell 1988a)
7.67 (HPLC-RT correlation, Hawker & Connell 1988)
7.729 ± 0.031 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
7.54 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
7.15 (recommended, Sangster 1993)
7.73 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.57, 10.38 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.77 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
5.82; 7.35 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.82, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
7.34 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.61, 5.46, 5.41, 4.99 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.610, 5.699 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, observed; calculated-MCI χ, Sabljic et al. 1989)
6.36, 6.13, 6.01 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
7.04 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 5070 d^{-1}; k_2 = 0.0077 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.006 d^{-1} with $t_{½}$ = 119 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 145 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 110 d for high-dose treatment, $t_{½}$ = 145 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.202.1
Reported aqueous solubilities and vapor pressures of 2,2′,3,3′,5,5′,6,6′-octachlorobiphenyl (PCB-202) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure	
Dickhut et al. 1986		Burkhard et al. 1984	
generator column-GC/ECD		gas saturation-GC/ECD	
t/°C	$S/g\cdot m^{-3}$	t/°C	P/Pa
20	1.29×10^{-4}	29.0	4.95×10^{-5}
25	1.29×10^{-4}	39.9	2.24×10^{-4}
32	2.15×10^{-4}	50.0	5.83×10^{-4}
50	7.73×10^{-4}	61.2	2.65×10^{-3}
		25.0	2.90×10^{-5}
$\ln x = A - B/(T/K)$			
A	−5.333	$\log (P/Pa) = A - B/(T/K)$	
B	6098.15	A	13.262
		B	5307.3
$\Delta H_{sol}/(kJ\ mol^{-1}) = 50.7 \pm 3.8$ for 25–50°C		temp range 29–61.2°C	
		$\Delta H_{subl}/(kJ\ mol^{-1}) = 101.7$	

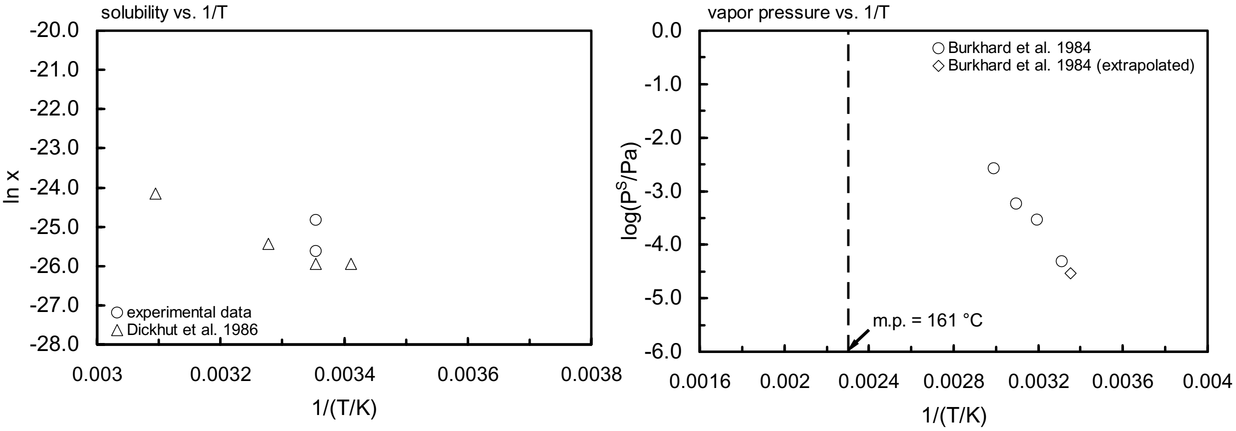
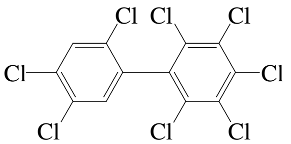


FIGURE 7.1.1.202.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,2′,3,3′,5,5′,6,6′-octachlorobiphenyl (PCB-202).

7.1.1.203 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl (PCB-203)



Common Name: 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl
Synonym: PCB-203, 2,2′,3,4,4′,5,5′,6-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl
CAS Registry No: 52663-76-0
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
2.91×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.36×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence):
1.35×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.52×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
9.29×10^{-5}, 1.047×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.47×10^{-5}, 5.62×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5244/(T/\text{K}) + 13.39$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.252 (calculated-P/C, Burkhard 1984)
14.21 (calculated-QSPR, Dunnivant et al. 1992)
0.990 (calculated-QSPR, Achman et al. 1993)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.57 (calculated-TSA, Burkhard 1984)
7.49 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.65 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.93 (generator column-GC, Larsen et al. 1992)
7.21 (recommended, Sangster 1993)
7.4825 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated :

12.36, 11.10	(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.24	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

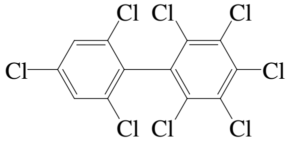
Sorption Partition Coefficient, log K_{OC}:

7.37	(suspended particulate matter, Burkhard 1984)
5.857	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

7.1.1.204 2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl (PCB-204)



Common Name: 2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl
Synonym: PCB-204, 2,2′,3,4,4′,5,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl
CAS Registry No: 74472-52-9
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
132 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
2.81×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.49×10^{-4}, 9.85×10^{-5}, 1.83×10^{-4}, 1.49×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.30×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.49×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.88×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.54×10^{-4}, 2.76×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.38×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4851/(T/K) + 12.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
53.3 (calculated-P/C, Burkhard 1984)
34.89 (calculated-QSAR, Dunnivant et al. 1992)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.59 (calculated-TSA, Burkhard 1984)
7.46, 7.63, 7.37, 7.45 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.30 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.48 (recommended, Sangster 1993)
7.2632 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
11.15 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

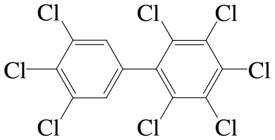
Sorption Partition Coefficient, log K_{OC}:

7.39	(suspended particulate matter, Burkhard 1984)
5.699	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

7.1.1.205 2,3,3′,4,4′,5,5′,6-Octachlorobiphenyl (PCB-205)



Common Name: 2,3,3′,4,4′,5,5′,6-Octachlorobiphenyl
Synonym: PCB-205, 2,3,3′,4,4′,5,5′,6-octachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5,5′,6-Octachlorobiphenyl
CAS Registry No: 74472-53-0
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
150 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
3.50×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
8.58×10^{-5} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
3.41×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.84×10^{-5} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
4.40×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
2.49×10^{-5}, 2.91×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -5402/(T/K) + 13.51$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
4.70 (calculated-P/C, Burkhard 1984)
8.644 (calculated-QSPR, Dunnivant et al. 1992)
10.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 169 \pm 6$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.47 (calculated-TSA, Burkhard 1984)
7.62 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
8.00 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.62 (recommended, Sangster 1993)
7.7326 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.86, 11.62 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.34 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.27	(suspended particulate matter, Burkhard 1984)
6.016	(marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 168$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

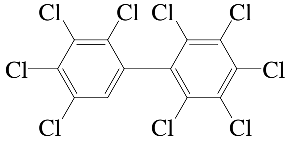
Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 166 d for high-dose treatment, $t_{½}$ = 168 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.206 2,2′,3,3′,4,4′,5,5′,6-Nonachlorobiphenyl (PCB-206)



Common Name: 2,2′,3,3′,4,4′,5,5′,6-Nonachlorobiphenyl
Synonym: PCB-206, 2,2′,3,3′,4,4′,5,5′,6-nonochloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,5′,6-nonachlorobiphenyl
CAS Registry No: 40186-72-9
Molecular Formula: $C_{12}HCl_9$
Molecular Weight: 464.213
Melting Point (°C):
204.5–206.5 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.507
Molar Volume (cm^3/mol):
372.7 (calculated-Le Bas method at normal boiling point)
276.1 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.70 (Opperhuizen et al. 1988; Ruelle et al. 1993)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.016 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.000112 (generator column-GC/ECD, Weil et al. 1974)
2.55×10^{-5} (generator column-GC/ECD, measured range 25–50°C, Dickhut et al. 1986)
2.55×10^{-5}, 5.117×10^{-5}, 6.59×10^{-5}, 1.32×10^{-4} (25, 32, 40, 50°C, generator column-GC/ECD, Dickhut et al. 1986)
$\ln x = -5990/(T/K) - 7.427$, temp range 25–50°C, ΔH_{ss} = 49.8 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
$\log x = -2609/(T/K) - 3.222$, ΔH_{ss} = 50.0 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
$S/(mol/L) = 1.27 \times 10^{-11} \exp(0.062 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
0.00011 (selected, Shiu & Mackay 1986)
3.07×10^{-5}, 3.14×10^{-5}, 2.61×10^{-5}, 2.80×10^{-5} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.80×10^{-5} (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
$\ln x = -7.4275 - 6004.5/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.88×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)
1.034×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
1.08×10^{-5}, 1.53×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -5226/(T/K) + 13.57$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
27.66 (calculated-P/C, Burkhard et al. 1985b)
8.845 (calculated-QSPR, Dunnivant et al. 1992)
0.474 (calculated-QSPR, Achman et al. 1993)

15.1 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
9.14 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
7.94, 7.91, 7.98, 7.94 (RP- HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.07 (generator column-GC, Larsen et al. 1992)
7.51 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
13.09, 11.79 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.81 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

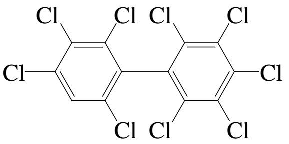
Bioconcentration Factor, log BCF:
5.71; 7.24 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
2.60–4.85 (various marine species, mean dry weight BCF, Hope et al. 1998)
4.37–5.67 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Sorption Partition Coefficient, log K_{OC}:
7.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.15, 5.92, 5.83, 5.69 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg L^{-1} DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
6.152; 6.133 (marine humic substances of 5 mg L^{-1} DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 4940$ d^{-1}; $k_2 = 0.00958$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.016$ d^{-1} with $t_{½} = 45$ d and $k_2 = 0.013$ d^{-1} with $t_{½} = 53$ d for food concn of 20 ng/g and 141 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.005$ d^{-1} with $t_{½} = 140$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005$ d^{-1} with $t_{½} = 148$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½} > 1000$ d in rainbow trout, and $t_{½} = 84$ d in its muscle (Niimi & Oliver 1983)
Depuration $t_{½}$.= 45–53 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{½} = 140$ d for high-dose treatment, $t_{½} = 148$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.207 2,2′,3,3′,4,4′,5,6,6′-Nonachlorobiphenyl (PCB-207)



Common Name: 2,2′,3,3′,4,4′,5,6,6′-Nonachlorobiphenyl
Synonym: PCB-207, 2,2′,3,3′,4,4′,5,6,6′-nonochloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,6,6′-nonachlorobiphenyl
CAS Registry No: 52663-79-3
Molecular Formula: $C_{12}HCl_9$
Molecular Weight: 464.213
Melting Point (°C):
 161 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
 372.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
 0.00167 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
 4.64×10^{-5}, 3.29×10^{-5}, 4.04×10^{-5}, 3.77×10^{-5} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 0.000058 (calculated-TSA, Abramowitz & Yalkowsky 1990)
 2.10×10^{-5} (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
 1.47×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985a)
 1.30×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
 3.17×10^{-5}, 4.99×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 $\log (P_L/\text{Pa}) = -5127/(T/\text{K}) + 12.70$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
 35.97 (calculated-P/C, Burkhard et al. 1985b)
 17.13 (calculated-QSPR, Dunnivant et al. 1992)
 0.717 (calculated-QSPR, Achman et al. 1993)
 97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 145 ± 7 kJ/mol, ΔS_H = 0.46 ± 0.04 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
 7.94 (calculated-TSA, Burkhard 1984)
 7.84, 7.97, 7.85, 7.86 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 7.52 (generator column-GC, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
 7.74 (calculated-TSA, Hawker & Connell 1988a)
 7.80 (calculated-MCI χ, Patil 1991)
 7.88 (recommended, Sangster 1993)
 7.6190 (calculated-molecular properties MNDO-AM1, Makino 1998)
 7.77 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.60, 11.26 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.94 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

2.65–4.54 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.02–6.29 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Sorption Partition Coefficient, log K_{OC}:

7.74 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.98, 5.77, 5.67, 5.44 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg L^{-1} DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.98, 5.97 (marine humic substances of 5 mg L^{-1} DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
6.39, 6.17, 6.19 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

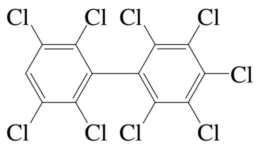
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 162$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 155$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½} = 162$ d for high-dose treatment, $t_{½} = 155$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.208 2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl (PCB-208)



Common Name: 2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl
Synonym: PCB-208, 2,2′,3,3′,4,5,5′,6,6′-nonochloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′,6,6′-nonachlorobiphenyl
CAS Registry No: 52663-77-1
Molecular Formula: $C_{12}HCl_9$
Molecular Weight: 464.213
Melting Point (°C):
180.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
372.7 (calculated-Le Bas method at normal boiling point)
276.1 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22.60 (Ruelle et al. 1993; Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
49.45 (Shiu & Mackay 1986)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0298 (mp at 180.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
1.80×10^{-5} (generator column-GC/ECD, Miller et al. 1984,1985)
6.87×10^{-5}; 4.64×10^{-5}, 6.87×10^{-5}, 3.95×10^{-5}, 4.97×10^{-5} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.74×10^{-7} (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.78×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)
1.22×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.08×10^{-5}, 6.62×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.19×10^{-5} (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -5127/(T/K) + 12.68$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
32.53 (calculated-P/C, Burkhard et al. 1985b)
16.93 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.92 (calculated-TSA, Burkhard 1984)
8.16 (generator column-GC/ECD, Miller et al. 1984,1985)
9.05 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
7.72, 7.87, 7,69, 7,78 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
8.18 (calculated-TSA, Hawker & Connell 1988a)

7.77 (recommended, Sangster 1993)
8.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.57, 11.26 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.71 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

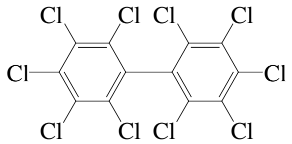
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
7.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.974 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.005$ d^{-1} with $t_{½} = 139$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005$ d^{-1} with $t_{½} = 152$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½} = 139$ d for high-dose treatment, $t_{½} = 152$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.209 2,2′,3,3′,4,4′,5,5′,6,6′-Decachlorobiphenyl (PCB-209)



Common Name: 2,2′,3,3′,4,4′,5,5′,6,6′-Decachlorobiphenyl
Synonym: PCB-209
Chemical Name: 2,2′,3,3′,4,4′,5,5′,6,6′-decachlorobiphenyl
CAS Registry No: 2051-24-3
Molecular Formula: $C_{12}Cl_{10}$
Molecular Weight: 498.658
Melting Point (°C):
309 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.507
Molar Volume (cm^3/mol):
393.6 (calculated-Le Bas method at normal boiling point)
289.0 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.79 (differential scanning calorimetry, Miller et al. 1984; Ruelle & Kesselring 1997)
39.434 (Ruelle et al. 1993)
38.16 (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
49.37 (Miller et al. 1984; Shiu & Mackay 1986; Hinckley et al. 1990)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00164 (mp at 309°C)
0.0017 (Mackay et al. 1980; Shiu & Mackay 1986; Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.015 (shake flask-GC/ECD, Wallnöfer et al. 1973; Tulp & Hutzinger 1978)
1.6×10^{-5} (generator column-GC/ECD, Weil et al. 1974)
7.43×10^{-6} (generator column-GC/ECD, Miller et al. 1984,1985)
2.12×10^{-8} (calculated-UNIFAC activity coeff., converted from log γ, Arbuckle 1986)
4.1×10^{-4}, 4.6×10^{-4} (exptl., calculated-UNIFAC, converted from log γ, Burkhard et al. 1986)
6.48×10^{-7}* (generator column-GC/ECD, measured range 50–80°C, Dickhut et al. 1986)
6.48×10^{-7}, 8.38×10^{-6}, 1.76×10^{-5}, 4.95×10^{-5} (25, 60, 70, 80°C, generator column-GC/ECD, Dickhut et al. 1986)
$\ln x = -8010.6/(T/K) - 4.608$, temp range 50–80°C, ΔH_{ss} = 66.6 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
$\log x = -3478/(T/K) - 2.001$, ΔH_{ss} = 66.6 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
$S/(mol/L) = 1.80 \times 10^{-13} \exp(0.077 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
7.37×10^{-6}, 8.67×10^{-6}, 7.04×10^{-6}, 9.07×10^{-6} (RP- HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
2.1×10^{-5} (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
$(7.9 \pm 0.38) \times 10^{-6}$ (generator column-SPME/GC, Paschke et al. 1998)
$\ln x = -4.632 - 8001/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.4×10^{-5} (calculated-volatilization rate, Dobbs & Cull 1982)
4.0×10^{-5} (supercooled liquid P_L, Mackay et al. 1983)

5.30×10^{-8}* (extrapolated, gas saturation-GC, measured range 50.7–89.8°C, Burkhard et al. 1984)
$\log (P/Pa) = 14.049 - 6358/(T/K)$; temp range 50.7–89.8°C (gas saturation, Burkhard et al. 1984)
1.39×10^{-6} (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
5.36×10^{-8} (GC-RI correlation, Burkhard et al. 1985a)
2.75×10^{-5} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
5.58×10^{-6}, 1.32×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.00×10^{-8}; 3.0×10^{-5} (selected, solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
9.44×10^{-6} (GC-RT correlation, Watanabe & Tatsukawa 1989)
5.14×10^{-6}, 1.44×10^{-5} (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
1.303×10^{-5} (P_{GC} by GC-RT correlation with *p,p′*-DDT as reference standard, Hinckley et al. 1990)
$\log (P_L/Pa) = 13.27 - 5402/(T/K)$ (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
$\log (P_L/Pa) = -5402/(T/K) + 13.27$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
$2.89 \times 10^{-9} - 1.40 \times 10^{-5}$; $(5.58–27.5) \times 10^{-6}$ (literature P_S range; P_L range, Delle Site 1997)
2.6×10^{-5}* (65°C, Knudsen effusion, measured range 65–85°C, Goodman 1997)

Henry's Law Constant (Pa m^3/mol at 25°C):
100 (estimated, Mackay et al. 1983)
12.46 (calculated-P/C, Burkhard et al. 1985b)
20.84 (calculated-P/C, Shiu & Mackay 1986; Shiu et al. 1987)
40.0 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
11.19 (Hansch & Leo 1979)
9.60 (TLC-RT correlation, Bruggeman et al. 1982; 1984)
8.26 (generator column-GC/ECD, Miller et al. 1984,1985)
8.20 (generator column-HPLC, Woodburn et al. 1984)
8.20 (shake flask/slow stirring-GC, Brooke et al. 1986)
8.20 (generator column-GC/ECD, Doucette & Andren 1987,1988)
8.38, 8.37, 8.41, 8.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
9.45, 11.2 (calculated-UNIFAC activity coeff., π const. or f const., Banerjee & Howard 1988)
8.274 ± 0.001(shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
> 9.0 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
8.24 (HPLC-retention indices correlation, Noegrohati & Hammers 1992)
8.27 (recommended, Hansch et al. 1995)
7.95 ± 0.68 (flask/slow stirring-SPME/GC, Paschke et al. 1998)
7.59 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
13.36, 1.96 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
12.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:
5.48 (guppy, 3.5% extractable lipid, Bruggeman et al. 1984; quoted, Gobas et al. 1987)
7.0 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
1.48, 1.41 (human fat of lipid basis, calculated-K_{OW}, Geyer et al. 1987)
1.38, 1.32 (human fat of wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
4.02 (guppy, Gobas et al. 1987; quoted, Banerjee & Baughman 1991)
4.02 (guppy, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)

5.07 (guppy, estimated, Banerjee & Baughman 1991)
5.44; 6.97 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
2.65–4.54 (various marine species, mean dry wt. BCF, Hope et al. 1998)
> 5.44, > 6.97 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
> 5.53, > 6.99 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
6.95, 8.26 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.32, 3.97 (human, steady-state not reached during whole life: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor, BSAF:
13 (trout in Lake Ontario, Niimi 1996)
0.047, 0.42, 0.10 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K_{OC}:
8.09 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.19, 5.99, 5.83, 5.61 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
6.19, 6.17 (marine humic substances of 5 mg L^{-1} DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization/Evaporation: 8.5×10^{-7} g m^{-1} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 40$ d^{-1}; $k_2 = 0.004$ d^{-1} (guppy, Bruggeman et al. 1984)
$k_1 = 600$ d^{-1} (guppy, Opperhuizen 1986)
log $k_1 = 1.60$ d^{-1}; log $1/k_2 = 2.39$ d (fish, quoted, Connell & Hawker 1988)
$k_1 = 3640$ d^{-1}; $k_2 = 0.0132$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.013$ d^{-1} with $t_{½} = 52$ d and $k_2 = 0.013$ d^{-1} with $t_{½} = 52$ d for food concn of 62 ng/g and 688 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.005$ d^{-1} with $t_{½} = 127$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005$ d^{-1} with $t_{½} = 149$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½} > 1000$ d in rainbow trout, and $t_{½} = 122$ d its muscle (Niimi & Oliver 1983);
$t_{½} = 175$ d in guppy (Bruggeman et al. 1984).
Depuration $t_{½} = 52$ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{½} = 127$ d for high-dose treatment, $t_{½} = 149$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.209.1
Reported aqueous solubilities and vapor pressures of decachlorobiphenyl at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure			
Dickhut et al. 1986		Burkhard et al. 1984		Goodman 1997	
generator column-GC/ECD		gas saturation-GC/ECD		Knudsen effusion	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
25	6.48×10^{-7}	50.7	2.69×10^{-6}	65	2.6×10^{-5}
60	8.38×10^{-6}	64.9	1.68×10^{-5}	70	5.1×10^{-5}
70	1.76×10^{-5}	72.3	4.00×10^{-5}	75	8.1×10^{-5}
80	4.95×10^{-5}	80.5	1.43×10^{-4}	80	1.10×10^{-4}
		85.2	1.88×10^{-4}	85	1.80×10^{-4}
ln x = A – B/(T/K)		89.8	3.36×10^{-4}		
A	–4.608	25.0	5.30×10^{-8}		
B	8010.6			log (P/Pa) = A – B/(T/K)	
		log (P/Pa) = A – B/(T/K)			
enthalpy of solution:			P/Pa	A	9.91
ΔH_{sol}/(kJ mol^{-1}) = 66.6 ± 4.9		A	14.049	B	4886
for 40–80°C		B	6358.0		
		temp range 50.7–89.8°C			
		ΔH_{subl}/(kJ mol^{-1}) = 101.7			

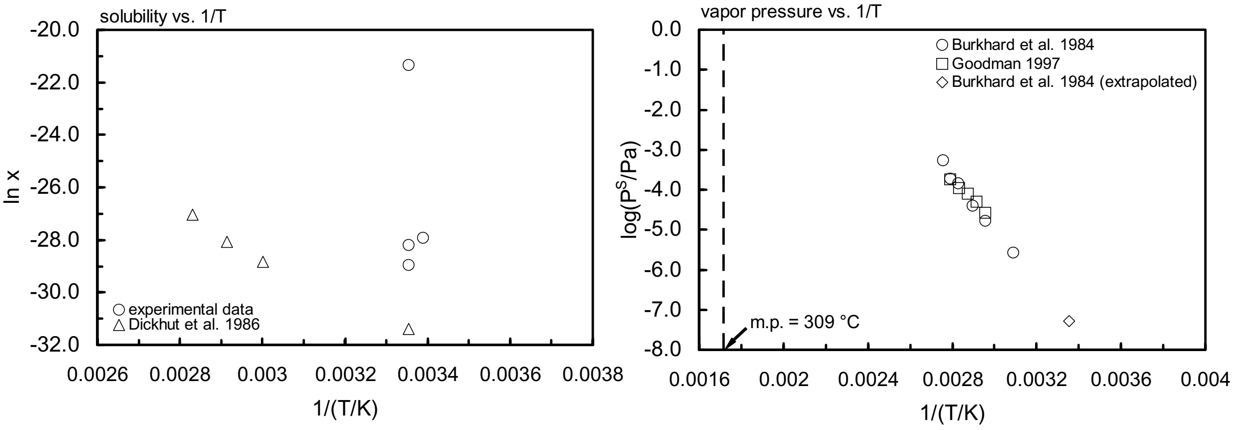


FIGURE 7.1.1.209.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,2′,3,3′,4,4′,5,5′,6,6′-decachlorobiphenyl (PCB-209).

7.1.2 ISOMER GROUPS

7.1.2.1 Monochlorobiphenyl

Common Name: Monochlorobiphenyl
Synonym: Dowtherm G
Chemical Name: monochlorobiphenyl
CAS Registry No: 27323-18-8
Molecular Formula: $C_{12}H_9Cl$
No. of Isomers: 3
Molecular Weight: 188.652
Melting Point (°C):
  25–77.9 (Shiu et al. 1987)
Boiling Point (°C): 285
Chlorine Content: 18.79% (Hutzinger et al. 1974)
Density (g/cm^3): 1.1
Molar Volume (cm^3/mol):
  205.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.30–1.0 (Mackay et al. 1983)
  0.301–1.0 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
  0.06–1.5 (selected, Mackay et al. 1983)
  7.20 (selected, supercooled liq., Mackay et al. 1983a)
  0.795–6.17, 4.08(exptl. range, calculated-UNIFAC, converted from log γ, Burkhard et al. 1986)
  1.2–5.5 (selected, Shiu et al. 1987)
  2.5–6.73 (selected, supercooled liquid, Shiu et al. 1987)
  1.2–9.5 (selected, Formica et al. 1988)
  4.0 (selected, Metcalfe et al. 1988)
  1.2–5.5 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
  1.1–5.6 (selected, Mackay et al. 1983a)
  2.30 (supercooled liquid P_L, Mackay et al. 1983a)
  1.32 (selected, supercooled liq., Bopp 1983)
  1.10 (average, liquid, Mackay 1986; Metcalfe et al. 1988)
  0.271–2.04 (selected, solid, Shiu et al. 1987)
  0.9–2.5 (selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
  79.3 (calculated-P/C, Bopp 1983)
  58–74 (calculated, Mackay et al. 1983a)
  60.0 (selected, Mackay et al. 1983a,b)
  42.56–75.55 (calculated, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
  4.66 (selected, Mackay et al. 1983b)
  4.70 (selected, Mackay 1986; Metcalfe et al. 1988)
  4.3–4.6 (selected, Shiu et al. 1987)
  4.73 (calculated-no. Cl atoms, Formica et al. 1988)
  4.50 (quoted, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

3.40 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

Half-Lives in the Environment:

Air: atmospheric photodegradation, 0.62–1.4 d (Dilling et al. 1983); calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radicals for mono-chlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for monochlorobiphenyls (Kwok et al. 1995).

Surface water: 1.4–4.9 d in Lake Michigan (Neely 1983); 2–3 d for river water (Bailey et al. 1983).

Groundwater:

Sediment:

Soil:

Biota:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: k = 0.25 g/m^2 h (Mackay 1986; Metcalfe et al. 1988).

Photolysis: $t_{½}$ = 0.62–1.4 d for photodegradation in the atmosphere (Dilling et al. 1983).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(exptl) = (2.8 – 5.3) × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(calc) = (3.1 – 4.7) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp., and the tropospheric lifetime was calculated to be 5–11 d for monochlorobiphenyls (Atkinson 1987)

k_{OH} (exptl) = (2.8 – 5.3) × 10^{-12} cm^3 molecule^{-1} s^{-1}, and k_{OH}(calc) = (3.2 – 4.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. for reaction with monochlorobiphenyls, the tropospheric lifetime was calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, 7 × 10^{-8} nmol cell^{-1}·h^{-1} (Furukawa et al. 1978; selected, NAS 1979); time for 50% biodegradation of an initial concentration of 1–100 μg/L by river dieaway test is about 2–5 d (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

7.1.2.2 Dichlorobiphenyl

Common Name: Dichlorobiphenyl
Synonym:
Chemical Name: dichlorobiphenyl
CAS Registry No: 25512-42-9
Molecular Formula: $C_{12}H_8Cl_2$
No. of Isomers: 12
Molecular Weight: 223.098
Melting Point (°C):
  24.4–149 (Shiu & Mackay 1986; Shiu et al. 1987; quoted, Metcalfe et al. 1988)
Boiling Point (°C):
  312 (Shiu & Mackay 1986)
Chlorine Content: 31.77%
Density (g/cm^3 at 20°C): 1.30
Molar Volume (cm^3/mol):
  226.4 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.06–1.5 (Mackay et al. 1983)
  0.059–1.0 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
  0.22 (quoted, Bopp 1983)
  0.06–1.5, 2.20 (solid, supercooled liquid, Mackay et al. 1983a)
  0.898–1.96, 1.60(exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
  1.6 (Mackay 1986; quoted, Metcalfe et al. 1988)
  0.06–2.0, 1.02–2.26(selected, solid, supercooled liquid, Shiu et al. 1987)
  0.06–2.0 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
  0.223 (quoted, supercooled liquid, Bopp 1983)
  0.60 (quoted, supercooled liquid, Mackay et al. 1983a)
  0.03–0.36 (Mackay et al. 1983)
  0.24 (average, liquid, Mackay 1986; Metcalfe et al. 1988)
  0.0018–0.279, 0.008–0.60 (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
  153.6 (calculated-P/C, Bopp 1983)
  60.0 (Mackay et al. 1983a,b)
  97.0 (calculated-P/C, Mackay et al. 1983a)
  17–92.2 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
  5.19 (Mackay et al. 1983a,b)
  5.10 (Mackay 1986; Metcalfe et al. 1988)
  4.9–5.3 (selected, Shiu et al. 1987)
  5.13 (calculated-chlorine atoms, Formica et al. 1988)
  5.10 (quoted mean value for isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
  3.89 (biota, Mackay et al. 1983b)
  3.80 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
  4.10 (calculated-MCI χ, Koch 1983)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half Lives, $t_{½}$:

Volatilization/Evaporation: k = 0.065 g m^{-2} h^{-1} (selected, Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (1.4 – 2.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 8–17 d at room temp. (Atkinson 1987)

k_{OH}(exptl) = (2.0 – 4.2) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, the tropospheric lifetime is calculated to be 3.4–7.2 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, 6 × 10^{-8} nmol $cell^{-1}·h^{-1}$ (Furukawa et al. 1978; quoted, NAS 1979);

$t_{½}$ ~ 2–3 d for degradation, using river water dieaway test (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the calculated rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 2–3 d (Bailey et al. 1983).

Groundwater:

Sediment:

Soil:

Biota:

7.1.2.3 Trichlorobiphenyl

Common Name: Trichlorobiphenyl
Synonym:
Chemical Name: trichlorobiphenyl
CAS Registry No: 25323-68-6
Molecular Formula: $C_{12}H_7Cl_3$
No. of Isomers: 24
Molecular Weight: 257.543
Melting Point (°C):
28–87 (Shiu & Mackay 1986; Metcalfe et al. 1988)
Boiling Point (°C):
337 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 41.4%
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.24–0.65 (Mackay et al. 1983)
0.244–0.651 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.05 (Neely 1980)
0.15–0.64, 0.67(solid, supercooled liquid, Mackay et al. 1983)
0.0654–1.09 (exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.65 (quoted, Mackay 1986; Metcalfe et al. 1988)
0.015–0.40 (selected, Shiu et al. 1987)
0.015–0.40 (quoted, Formica et al. 1988)
0.015–0.40 (quoted range for individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
0.200 (Neely 1980)
0.0375 (supercooled liquid, Bopp 1983)
0.01–0.27, 0.20(solid, supercooled liquid, quoted, Mackay et al. 1983)
0.054 (average, liquid, Mackay 1986; Metcalfe et al. 1988)
0.0136–0.143, 0.003–0.022 (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
81.76 (calculated-P/C, Bopp 1983)
82–102 (calculated-P/C, Mackay et al. 1983)
77 (selected, Mackay et al. 1983)
24.3–92.2 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
5.76 (Mackay et al. 1983)
5.50 (Mackay 1986; Metcalfe et al. 1988)
5.5–5.9 (selected, Shiu et al. 1987)
5.53 (calculated-chlorine atoms, Formica et al. 1988)
5.80 (quoted mean value of isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
4.20 (fish, Mackay 1986; Metcalfe et al. 1988)
4.70 (calculated-MCI χ, Koch 1983)

Sorption Partition Coefficient, log K_{OC}:

Sorption Partition Coefficient, log K_P:

3.34	(lake sediment, calculated, Formica et al. 1988)
3.50	(calculated-MCI χ, Koch 1983)

Environmental Fate Rate Constants, k, or Half Lives, $t_{½}$:

Volatilization/Evaporation: k = 0.017 g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.7 - 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 14–30 d at room temp. (Atkinson 1987)

k_{OH}(calc) = $(1.0 - 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radicals for trichlorobiphenyls, the tropospheric lifetime is calculated to be 6.9–15 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, 5×10^{-8} nmol $cell^{-1} \cdot h^{-1}$ (Furukawa et al. 1978; quoted, NAS 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: estimated $t_{½}$ = 134 h from fish in simulated ecosystem (Neely 1980).

7.1.2.4 Tetrachlorobiphenyl

Common Name: Tetrachlorobiphenyl
Synonym:
Chemical Name: tetrachlorobiphenyl
CAS Registry No: 26914-33-0
Molecular Formula: $C_{12}H_6Cl_4$
No. of Isomers: 42
Molecular Weight: 291.988
Melting Point (°C):
47–180 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
360 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 48.6%
Density (g/cm^3 at 20°C): 1.5
Molar Volume (cm^3/mol):
268.2 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.1–0.68 (Mackay et al. 1983)
0.029–0.606 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.05 (Neely 1980)
0.0008–0.17 (Mackay et al. 1983)
0.017 (McCall et al. 1983)
0.02–0.0955, 0.224 (exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.26 (quoted, Mackay 1986; Metcalfe et al. 1988)
0.0043–0.10 (selected, Shiu et al. 1987)
0.039–0.38 (selected, supercooled liquid, Shiu et al. 1987)
0.001–0.10 (Formica et al. 1988)
0.001–0.10 (quoted range for individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
0.0653 (Neely 1980)
0.0064 (supercooled liquid, Bopp 1983)
0.003–0.104 (Mackay et al. 1983)
0.06 (supercooled liquid, Mackay et al. 1983)
0.0653 (McCall et al. 1983)
0.012 (Mackay 1986; Metcalfe et al. 1988)
$5.9 \times 10^{-5} - 5.4 \times 10^{-3}$ (selected, Shiu et al. 1987)
0.002 (selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
34.69 (calculated-P/C, Bopp 1983)
75–94 (calculated-P/C, Mackay et al. 1983)
76.0 (Mackay et al. 1983)
1.72–47.59 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
6.35 (suggested, Mackay et al. 1983)
5.90 (Mackay 1986, Metcalfe et al. 1988)
5.6–6.5 (selected, Shiu et al. 1987)

5.93	(calculated-chlorine atoms, Formica et al. 1988)
6.00	(quoted mean value for isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

3.98	(pinfish, Branson et al. 1975; quoted, Waid 1986)
3.95	(trout, Branson et al. 1975; quoted, NAS 1979)
4.79	(McCall et al. 1983)
4.60	(fish, Mackay 1986; Metcalfe et al. 1988)
5.30	(calculated-MCI χ, Koch 1983)

Sorption Partition Coefficient, log K_{OC}:

4.51	(correlated, McCall et al. 1983)
3.43–5.11	(correlated of literature values in high clay soils, Sklarew & Girvin 1987)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: k = 4.2×10^{-3} g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 25–60 d at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radicals for tetrachlorobiphenyls, the tropospheric lifetime is calculated to be 8.5–40 d (Kwok et al. 1995).

Hydrolysis:

Biodegradation: rate of degradation for both rings substituted with chlorine using species of Alcaligenes and Acinetobacter, 2.5×10^{-8} nmol $cell^{-1}$ h^{-1} (Furukawa et al. 1978; selected, NAS 1979);

no degradation by river dieaway test after 98 d of incubation (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil: volatilization $t_{1/2}$ ~ 10 d from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).

Biota: estimated $t_{1/2}$ = 139 h from fish in simulated ecosystem (Neely 1980).

7.1.2.5 Pentachlorobiphenyl

Common Name: Pentachlorobiphenyl
Synonym:
Chemical Name: pentachlorobiphenyl
CAS Registry No: 25429-29-2
Molecular Formula: $C_{12}H_5Cl_5$
No. of Isomers: 46
Molecular Weight: 326.433
Melting Point (°C):
  –23.5–124 (Shiu et al. 1987)
  76.5–124 (Shiu & Mackay 1986; Metcalfe et al. 1988)
Boiling Point (°C):
  381 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 54.4%
Density (g/cm^3 at 20°C): 1.50
Molar Volume (cm^3/mol):
  289.1 (Le Bas method at normal boiling point, Shiu & Mackay 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.1–0.31 (Mackay et al. 1983)
  0.105–0.311 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
  0.01 (Neely 1980)
  0.004–0.03 (Mackay et al. 1983)
  0.072 (supercooled liquid, Mackay et al. 1983)
  0.0338–0.0525, 0.0829 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
  0.099 (Mackay 1986; Metcalfe et al. 1988)
  0.004–0.02 (selected, Shiu et al. 1987)
  0.03–0.11 (selected, supercooled liquid, Shiu et al. 1987)
  0.004–0.02 (Formica et al. 1988)
  0.024 (selected average value of isomers, Mackay 1989)
  0.004–0.02 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
  0.01026 (Neely 1980)
  0.00111 (supercooled liquid, Bopp 1983)
  0.015 (supercooled liquid, Mackay et al. 1983)
  0.004–0.03 (Mackay et al. 1983)
  0.0026 (Mackay 1986; Metcalfe et al. 1988)
  0.000304–0.0093(selected, Shiu et al. 1987)
  0.0023–0.051(selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
  68.0 (suggested, Mackay et al. 1983)
  17.34 (calculated-P/C, Bopp 1983)
  24.8–151.4 (selected, Shiu et al. 1987)
  12.2 (calculated, Mackay 1989)

Octanol/Water Partition Coefficient, log K_{OW}:
  6.85 (suggested, Mackay et al. 1983)
  6.33 (calculated-chlorine atoms, Formica et al. 1988)

6.30	(Mackay 1986; Metcalfe et al. 1988)
6.2–6.5	(selected, Shiu et al. 1987)
6.60	(selected, Mackay 1989)
6.40	(quoted mean value for isomers of a homolog group, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

5.0	(fish, Mackay 1986; Metcalfe et al. 1988)
5.30	(Mackay 1989)
5.90	(calculated-MCI χ, Koch 1983)

Sorption Partition Coefficient, log K_{OC}:

6.21	(calculated, $0.41K_{OW}$, Mackay 1989)

Sorption Partition Coefficient, log K_P:

4.15	(lake sediment, calculated-K_{OW}, f_{OC}, Formica et al. 1988)
4.51	(calculated-MCI χ, Koch 1983)

Environmental Fate Rate Constants, k, and Half Lives, $t_{1/2}$:

Volatilization /Evaporation: $k = 1.0 \times 10^{-3}$ g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2 - 0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp., with a calculated tropospheric lifetime of 60–120 d (Atkinson 1987);

k_{OH}(calc) = $(0.3 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radicals for pentachlorobiphenyls, the tropospheric lifetime is calculated to be 16–48 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.62–1.4 d for atmospheric photodegradation (Dilling et al. 1983);

calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radicals for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radicals for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil: volatilization $t_{1/2}$ = 25 d from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).

Biota: estimated $t_{1/2}$ = 226 d from fish in simulated ecosystem (Neely 1980).

7.1.2.6 Hexachlorobiphenyl

Common Name: Hexachlorobiphenyl
Synonym:
Chemical Name: hexachlorobiphenyl
CAS Registry No: 26601-64-9
Molecular Formula: $C_{12}H_4Cl_6$
No. of Isomers: 42
Molecular Weight: 360.878
Melting Point (°C):
  85–160 (Shiu et al. 1987)
  77–150 (Shiu & Mackay 1986; Metcalfe et al. 1988)
Boiling Point (°C):
  400 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 62.77% (Hutzinger et al. 1974)
Density (g/cm^3 at 20°C): 1.60
Molar Volume (cm^3/mol):
  310.0 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.06–0.25 (Mackay et al. 1983)
  0.0582–0.256(Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
  0.0004–0.01, 0.021 (solid, supercooled liquid, Mackay et al. 1983)
  0.00303–0.0504, 0.00297 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
  0.038 (Mackay 1986; Metcalfe et al. 1988)
  0.0004–0.001, 0.0022–0.01 (solid, supercooled liquid, Shiu et al. 1987)
  0.0004–0.005 (Formica et al. 1988)
  0.0035 (Mackay & Paterson 1991)
  0.0004–0.001 (quoted range, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
  0.000182 (supercooled liquid, Bopp 1983)
  0.0016, 0.005 (solid, supercooled liquid, Mackay et al. 1983)
  5.8×10^{-4} (Mackay 1986; Metcalfe et al. 1988)
  $2.0 \times 10^{-5} - 1.59 \times 10^{-3}$, $7.0 \times 10^{-4} - 0.012$ (solid, supercooled liquid, Shiu et al. 1987)
  0.0005 (selected, Mackay & Paterson 1991)

Henry's Law Constant (Pa m^3/mol at 25°C):
  86.0 (Mackay et al. 1983)
  6.70 (calculated-P/C, Bopp 1983)
  11.9–81.8 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
  6.70–7.30 (selected, Shiu et al. 1987)
  6.70 (selected, Mackay 1986; Metcalfe et al. 1988)
  6.80 (selected, Mackay & Paterson 1991)
  7.00 (quoted mean value for isomers of a homolog group, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
  6.50 (calculated-MCI χ, Koch 1983)
  5.39 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
  4.57 (green alga, Mailhot 1987)

Sorption Partition Coefficient, log K_{OC}:

4.785–6.869 (correlated literature values in high clay soils, Sklarew & Girvin 1987)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: 2.5×10^{-4} g m^{-2} h^{-1} (Mackay 1986; Metcalf et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp., the tropospheric lifetime is calculated to be 29–60 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: degradation rate constants estimated to be 1.5×10^{-5} h^{-1} in water, soil and sediment (Mackay & Patterson 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil: volatilization $t_{½}$ = 40 d from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).

Biota:

7.1.2.7 Heptachlorobiphenyl

Common Name: Heptachlorobiphenyl
Synonym:
Chemical Name: heptachlorobiphenyl
CAS Registry No: 28655-71-2
Molecular Formula: $C_{12}H_3Cl_7$
No. of Isomers: 24
Molecular Weight: 395.323
Melting Point (°C):
122.4–149 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
417 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 62.77% (Hutzinger et al. 1974)
Density (g/cm^3 at 20°C): 1.70
Molar Volume (cm^3/mol):
330.9 (Le Bas method at normal boiling point, Shiu & Mackay 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0596–0.109(Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0005, 0.006 (solid, supercooled liquid, Mackay et al. 1983)
0.00816–0.0205, 0.011 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.014 (Mackay 1986; Metcalfe et al. 1988)
0.00045–0.002, 0.0076–0.018 (solid, supercooled liquid, selected, Shiu et al. 1987)
0.00046–0.002(Formica et al. 1988)

Vapor Pressure (Pa at 25°C):
0.0015 (supercooled liquid, Mackay et al. 1983)
1.3×10^{-4} (Mackay 1986; Metcalfe et al. 1988)
2.73×10^{-5}, 2.5×10^{-4} (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol):
100.0 (Mackay et al. 1983)
5.4 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
7.1 (Mackay 1986; Metcalfe et al. 1988)
6.7–7.0 (selected, Shiu et al. 1987)

Bioconcentration Factor, log BCF:
7.10 (calculated-MCI χ, Koch 1983)
5.80 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization/Evaporation: $k = 6.2 \times 10^{-5}$ g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis:

Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

7.1.2.8 Octachlorobiphenyl

Common Name: Octachlorobiphenyl
Synonym:
Chemical Name: octachlorobiphenyl
CAS Registry No: 31472-83-0
Molecular Formula: $C_{12}H_2Cl_8$
No. of Isomers: 12
Molecular Weight: 429.768
Melting Point (°C):
 159–162 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
 432 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 65.98% (Hutzinger et al. 1974)
Density (g/cm^3 at 20°C): 1.7
Molar Volume (cm^3/mol):
 351.8 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
 0.0443–0.0474(Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
 0.0002–0.007, 0.020 (solid, supercooled liquid, estimated, Mackay et al. 1983)
 0.00345–0.006, 0.00378 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
 0.0055 (Mackay 1986; Metcalfe et al. 1988)
 0.0002–0.0003, 0.004–0.0068 (solid, supercooled liquid, Shiu et al. 1987)

Vapor Pressure (Pa at 25°C):
 2.8×10^{-5} (Mackay 1986; Metcalfe et al. 1988)
 2.66×10^{-5}, 6.0×10^{-3} (solid, supercooled liquid, selected, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
 100.0 (suggested, Mackay et al. 1983)
 38.08 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
 8.55 (Mackay et al. 1983)
 7.50 (Mackay 1986; Metcalfe et al. 1988)
 7.1 (selected, Shiu et al. 1987)

Bioconcentration Factor, log BCF:
 6.20 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:
 Volatilization/Evaporation: $k = 1.5 \times 10^{-5}$ g m^{-2}·h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Half-Lives in the Environment:

7.1.2.9 Nonachlorobiphenyl

Common Name: Nonachlorobiphenyl
Synonym:
Chemical Name: nonachlorobiphenyl
CAS Registry No: 53742-07-7
Molecular Formula: $C_{12}HCl_9$
No. of Isomers: 3
Molecular Weight: 464.213
Melting Point (°C):
182.8–206 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
445 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 68.73% (Hutzinger et al. 1974)
Density (g/cm^3 at 20°C): 1.80
Molar Volume (cm^3/mol):
372.7 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.016 (Mackay et al. 1983)
0.0163–0.0276(Shiu et al. 1987)

Solubility (g/m^3 or mg/L at 25°C):
0.0001, 0.0007 (solid, supercooled liquid, Mackay et al. 1983)
0.000678–0.00148, 0.00145 (exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.002 (Mackay 1986; Metcalfe et al. 1988)
0.000018–0.00011, 0.00065–0.0068 (solid, supercooled liquid, selected, Shiu et al. 1987)

Vapor Pressure (Pa at 25°C):
0.00015 (supercooled liquid, Mackay et al. 1983)
6.3×10^{-6} (Mackay 1986; Metcalfe et al. 1988)

Henry's Law Constant (Pa m^3/mol at 25°C):
100.0 (estimated, Mackay et al. 1983)

Octanol/Water Partition Coefficient, log K_{OW}:
9.14 (Mackay et al. 1983)
7.9 (Mackay 1986; Metcalfe et al. 1988)
7.2–8.16 (selected, Shiu et al. 1987)

Bioconcentration Factor, log BCF:
6.60 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:
Volatilization/Evaporation: $k = 3.5 \times 10^{-6}$ g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Half-Lives in the Environment:

7.1.3 AROCLOR MIXTURES

7.1.3.1 Aroclor 1016

Common Name: Aroclor 1016
Synonym:
Chemical Name:
CAS Registry No: 12674-11-2
Molecular Formula:
Average Molecular Weight: 257
Physical state: mobile oil
Distillation Range (°C):

323–356	(NAS 1979; Brinkman & De Kock 1980)

Chlorine Content: 41%
Density (g/cm^3):

1.37	(20°C, Brinkman & De Kock 1980)
1.36–1.37	(25°C, NAS 1979)
1.33	(Mills et al. 1982)
1.40	(25°C, Mackay 1986)

Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

0.22–0.25	(estimated, Tucker et al. 1975)
0.906	(23°C, shake flask-GC/ECD, Griffin et al. 1978; quoted, Lee et al. 1979)
0.42	(shake flask-GC/ECD, Paris et al. 1978; Callahan et al. 1979; Mackay et al. 1980; Mills et al. 1982)
0.906	(shake flask-GC/ECD, Lee et al. 1979)
0.049, 0.490	(shake flask, nephelometric, Hollifield 1979)
0.085	(Kenaga & Goring 1980)
0.34	(quoted, Pal et al. 1980)
0.906	(23°C, shake flask-GC/ECD, Griffin & Chian 1981; quoted, Sklarew & Girvin 1987)
0.40–0.91	(selected, Mackay et al. 1983)
0.84	(selected, Mackay 1986; Metcalfe et al. 1988)
0.332	(quoted, Chou & Griffin 1986)

Vapor Pressure (Pa at 25°C):

0.0533	(Monsanto Co. 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)
0.060	(quoted, Mackay et al. 1983)
0.200	(quoted, supercooled liquid, Mackay et al. 1983)
0.10	(selected, Mackay 1986; Metcalfe et al. 1988)
0.12, 0.121	(GC-RT correlation, Foreman & Bidleman 1985)

Henry's Law Constant (Pa m^3/mol at 25°C):

1368	(calculated, Paris et al. 1978)
33.4	(calculated-P/C, Mabey et al. 1982)
77.0	(calculated, Mackay et al. 1983)

Octanol/Water Partition Coefficient, log K_{OW}:

> 5.58	(shake flask, Chiou et al. 1977; Callahan et al. 1979; Veith et al. 1979a; Kenaga & Goring 1980; Mabey et al. 1982; Mackay 1982)
4.38	(shake flask-GC, Paris et al. 1978; quoted, Callahan et al. 1979; Ryan et al. 1988)
5.88	(HPLC-RT correlation, Veith et al. 1979b; Garten & Trabalka 1983)
3.48	(Pal et al. 1980; Sklarew & Girvin 1987)

4.3–5.48 (quoted, Mills et al. 1982)
4.40–5.80 (selected, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988)
5.31 (quoted, Chou & Griffin 1986)

Bioconcentration Factor, log BCF:

3.80, 3.81, 3.74 (bacteria: Doe Run pond, Hickory Hills pond, USDA pond, Paris et al. 1978)
4.18 (fish in Hudson River, Skea et al. 1979; quoted, Waid 1986)
4.63 (fathead minnow, 32-d exposure, Veith et al. 1979b; Veith & Kosian 1983)
4.69, 3.81 (fish, flowing water, static water, Kenaga & Goring 1980)
4.69 (quoted, Bysshe 1982)
4.70 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
4.63; 4.56 (fish, quoted; calculated-K_{OW}, Mackay 1982)
0.15 (rodents, Garten & Trabalka 1983)
4.63 (fish, Garten & Trabalka 1983)
4.63 (fathead minnow, quoted, Zaroogian et al. 1985)
4.24, 4.30 (oyster, quoted, Zaroogian et al. 1985)
3.11–4.5 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

5.19, 5.23, 4.96, 4.73 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
5.26 (calculated-K_{OW}, Mabey et al. 1982)
4.87 (calculated, Sklarew & Girvin 1987)
4.25 (soil, calculated-S, Chou & Griffin 1986)
5.03, 4.97 (sediments: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: volatilization $t_{1/2}$ = 9.9 h (Paris et al. 1978, quoted Callahan et al. 1979); rate constant k = 0.031 g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, k << 360 M^{-1} h^{-1} and k << 1 M^{-1} h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: 32.9% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972);
33% degraded by activated sludge for 48-h exposure (Tucker et al. 1975; Versar Inc. 1979; quoted, Pal et al. 1980);
rate constant k = 0.2 d^{-1} by acclimated activated sludge with $t_{1/2}$ = 3.5 d (Callahan et al. 1979).
96% loss by degradation with Nocardia strain NCIB 10603 and 91% loss with NCIB 10643, both within 52 d; > 98% loss with NCIB 10603 and > 96% loss with NCIB 10643, both within 100 d (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation: k ~ 3×10^{-9} to 3×10^{-12} mL $cell^{-1}$ h^{-1}, estimated for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ = 9.9 h in 1 m^3 water of 1-m deep (Paris et al. 1978; selected, Callahan et al. 1979; Mills et al. 1982)

Groundwater:

Sediment:

Soil: $t_{1/2}$ > 50 d (Ryan et al. 1988).

Sludge: estimated $t_{1/2}$ = 15 d for the volatilization from activated sludge under aerobic conditions (Tucker et al. 1975; quoted, Pal et al. 1980).

Biota: $t_{1/2}$ ~ 1.2 yr in fish in Hudson River (Armstrong & Sloan 1985).

7.1.3.2 Aroclor 1221

Common Name: Aroclor 1221
Synonym:
Chemical Name:
CAS Registry No: 11104-28-2
Molecular Formula:
Average Molecular Weight: 192–200.7
Physical State: mobile oil
Distillation Range (°C):

275–320	(NAS 1979; Brinkman & De Kock 1980)

Chlorine Content: 20.5–21.5%
Density (g/cm^3):

1.182–1.19	(25°C, NAS 1979)
1.18	(20°C, Brinkman & De Kock 1980)
1.15	(Callahan et al. 1979; Mills et al. 1982)

Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

5.00	(Zitko 1970, 1971)
3.5	(23°C, shake flask-GC/ECD, Griffin et al. 1978; quoted, Chou & Griffin 1986)
15.0	(Monsanto Co. 1972; quoted, Callahan et al. 1979; Pal et al. 1980; Mills et al. 1982)
3.52	(shake flask-GC/ECD, Lee et al. 1979)
0.59	(shake flask-nephelometric, Hollifield 1979)
40.0	(calculated-K_{OW}, Mabey et al. 1982)
3.50–15.0	(selected, Mackay et al. 1983)

Vapor Pressure (Pa at 25°C):

0.893	(Monsanto Co. 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)
0.93	(Pal et al. 1980)
0.89	(quoted, Mackay et al. 1983)

Henry's Law Constant (Pa m^3/mol):

0.750	(Hetling et al. 1978)
17.23	(calculated-P/C, Mabey et al. 1982)
60.0	(suggested value, Mackay et al. 1983)
23.10	(calculated, Burkhard et al. 1985b)

Octanol/Water Partition Coefficient, log K_{OW}:

2.8	(Monsanto Co. 1972; quoted, Callahan et al. 1979)
2.81	(Pal et al. 1980)
4.08	(Callahan et al. 1979; Mabey et al. 1982)
4.10–4.70	(quoted, Mackay et al. 1980)
2.78–4.0	(quoted, Mills et al. 1982)
4.09	(quoted, Chou & Griffin 1986)
4.09	(quoted, Ryan et al. 1988)

Bioconcentration Factor, log BCF:

3.34	(microorganism, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

3.76	(sediment, calculated-K_{OW}, Mabey et al. 1982)
3.62	(soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated k ~ 1.74 mg cm^{-2} h^{-1} from liquid substrate at 100°C (Hutzinger et al. 1974; quoted, Pal et al. 1980).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, k << 360 M^{-1} h^{-1} and k << 1 M^{-1} h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: 80.6% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980);
81% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980);
k = 0.8 d^{-1} and $t_{½}$ = 0.9 d for biodegradation by acclimated activated sludge (Callahan et al. 1979).

Biotransformation: estimated k ~ 3×10^{-9} to 3×10^{-12} mL $cell^{-1}$ h^{-1} rate of transformation for bacteria in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil: $t_{½}$ > 50 d (Ryan et al. 1988).

Sludge: estimated $t_{½}$ = 12 d of volatilization from activated sludge to be 12 d under aerobic conditions (Tucker et al. 1975; quoted, Pal et al. 1980).

Biota:

7.1.3.3 Aroclor 1232

Common Name: Aroclor 1232
Synonym:
Chemical Name:
CAS Registry No: 11141-16-5
Molecular Formula:
Average Molecular Weight: 221–232.2
Physical State: mobile oil
Distillation Range (°C):
270–325 (NAS 1979; Brinkman & De Kock 1980)
Chlorine Content: 32%
Density (g/cm^3):
1.260 (20°C, Brinkman & De Kock 1980)
1.27–1.28 (25°C, NAS 1979)
1.24 (Callahan et al. 1979; Mills et al. 1982)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
1.45 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Chou & Griffin 1986)
1.45 (quoted, Pal et al. 1980; Mackay et al. 1983)
407 (calculated-K_{OW}, Mabey et al. 1982)

Vapor Pressure (Pa at 25°C):
0.54 (Monsanto Co. 1972; Callahan et al. 1979; Mabey et al. 1982)
0.533 (quoted, Mills et al. 1982)
0.54 (quoted, Mackay et al. 1983)

Henry's Law Constant (Pa m^3/mol):
60.0 (suggested, Mackay et al. 1980)
1.14 (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:
3.2 (Monsanto Co. 1972; Callahan et al. 1979; Mabey et al. 1982)
4.54 (Tulp & Hutzinger 1978; Callahan et al. 1979)
3.23 (quoted, Pal et al. 1980)
3.18–4.48 (quoted, Mills et al. 1982)
4.10–5.20 (quoted, Mackay et al. 1983)
4.62 (calculated-S, Chou & Griffin 1986)
4.54 (quoted, Ryan et al. 1988)

Bioconcentration Factor, log BCF:
2.54 (microorganism, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
2.89 (sediment, calculated-K_{OW}, Mabey et al. 1982)
3.85 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen k << 360 M^{-1} h^{-1} and k << 1 $M^{-1}\cdot h^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: aerobic biodegradation $t_{½}$ = 61.4 d without the addition of polymer chitin, $t_{½}$ = 33.4 d with chitin and $t_{½}$ = 26.8 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: k ~ 3×10^{-9} to 3×10^{-12} $mL\cdot cell^{-1}\cdot h^{-1}$, estimated rate of transformation for bacteria in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: aerobic biodegradation $t_{½}$ = 61.4 d without the addition of polymer chitin, $t_{½}$ = 33.4 d with chitin and $t_{½}$ = 26.8 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Groundwater:

Sediment:

Soil: $t_{½}$ > 50 d (Ryan et al. 1988).

Biota:

7.1.3.4 Aroclor 1242

Common Name: Aroclor 1242
Synonym:
Chemical Name:
CAS Registry No: 534-692-19
Molecular Formula:
Average Molecular Weight: 261–266.5
Physical State: mobile oil
Distillation Range (°C):

325–366	(NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)

Chlorine Content: 42%
Density (g/cm^3):

1.38	(Brinkman & De Kock 1980)
1.30–1.39	(quoted, NAS 1979)
1.35	(Callahan et al. 1979; Mills et al. 1982)
1.40	(quoted, Mackay 1986; Metcalfe et al. 1988)

Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.20	(Monsanto Co. 1972; quoted, Hutzinger et al. 1974; Tucker et al. 1975 Sawhney 1987)
0.20	(20°C, Nisbet & Sarofim 1972)
0.24	(quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Brinkman & De Kock 1980; Geyer et al. 1980; Pal et al. 1980; Erickson 1986)
0.045	(shake flask-GC, Lawrence & Tosine 1976)
0.085	(Branson 1977; Kenaga & Goring 1980)
0.703	(23°C, shake flask-GC/ECD, Griffin et al. 1978)
0.34	(shake flask-GC/ECD, Paris et al. 1978)
0.1329	(11.5°C, shake flask-GC/ECD, Dexter & Pavlou 1978)
0.23	(quoted, Callahan et al. 1979; Mabey et al. 1982)
0.23–0.703	(shake flask-GC, Lee et al. 1979)
0.10	(shake flask-nephelometric, Hollifield 1979)
0.703	(20°C, Griffin & Chian 1980; quoted, Sklarew & Girvin 1987)
0.25	(quoted, Eisenreich et al. 1981)
0.34–0.703	(selected, Westcott et al. 1981)
0.10–0.30	(selected, Mills et al. 1982)
0.75	(selected, Mackay 1986; Metcalfe et al. 1988)
0.277	(20°C, calculated from mole fraction, Murphy et al. 1987)
0.097; 0.085–0.34	(21°C, shake flask-GC/ECD; quoted lit. range, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.0133	(20°C, Nisbet & Sarofim 1972)
0.12	(20°C, extrapolated, Monsanto 1972; NAS 1979)
log (P_L/mmHg) = 8.80 – 3500/(T/K) (temp range 150–300°C, from Monsanto 1972, NAS 1979)	
0.055	(quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983; Bidleman & Christinsen 1979)
0.054	(Callahan et al. 1979; Westcott et al. 1981; Eisenreich et al. 1981; Richardson et al. 1983)
0.054	(Pal et al. 1980; quoted, Sklarew & Girvin 1987)
0.040	(38°C, average, Wingender & Williams 1984)
0.076, 0.077	(GC-RT correlation, Foreman & Bidleman 1985)
0.077	(quoted, Mackay et al. 1986)
0.0517	(quoted, Eisenreich 1987)

0.091 (selected, Mackay 1986; Metcalfe et al. 1988)
0.033 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
58.06 (calculated, Mackay & Leinonen 1975)
768 (calculated, Paris et al. 1978)
59.5 (Slinn et al. 1978)
56.74 (calculated-P/C, Eisenreich et al. 1981)
20.32–41.62 (Westcott et al. 1981)
20.27–41.54 (calculated, Westcott et al. 1981)
79.02 (batch stripping, Atlas et al. 1982; quoted, Eisenreich et al. 1983; Atlas & Giam 1986)
34.69 (radiotracer-equilibration, Atlas et al. 1982; Atlas & Giam 1986)
200.6 (calculated-P/C, Mabey et al. 1982)
22.29 (direct concn. ratio-GC/ECD, Murphy et al. 1983)
40.3 (16°C, calculated-P/C, Richardson et al. 1983)
34.75 (calculated, Burkhard et al. 1985b)
50.0 (calculated, Mackay et al. 1986)
34.45 (calculated-P/C, Eisenreich 1987)
23.0 (20°C, quoted, Murphy et al. 1987 from Burkhard et al. 1985b)
28.31 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
28.27 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 12.869 - 4339/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
4.11 (Callahan et al. 1979; Mabey et al. 1982; quoted, Ryan et al. 1988)
5.58 (HPLC-RT correlation, Veith et al. 1979a; quoted, Kenaga & Goring 1980)
0.703 (shake flask-GC/ECD, Lee et al. 1979)
3.54 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
4.0–5.6 (quoted, Mills et al. 1982)
4.50–5.80 (quoted, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
5.90 (Rapaport & Eisenreich 1984)
5.74 (literature mean, Di Toro et al. 1985)
5.29 (quoted, Chou & Griffin 1986)

Bioconcentration Factor, log BCF:
3.92, 3.65, 3.46(bacteria: Doe Run pond, Hickory Hills pond, USDA pond, Paris et al. 1978)
0.08, –0.22 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
4.69, 3.81 (fish, flowing water, static water, Kenaga & Goring 1980)
4.69 (quoted, Bysshe 1982)
3.36 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
0.30, 0.13, –0.11, –0.50, –0.27 (rodent, poultry, sheep, small birds, swine, Garten & Trabalka 1983)
3.20–4.51 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
4.69, 5.99 (fish 5% lipid in flow-through system: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:
5.13, 5.18, 4.89, 4.70 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
3.80 (sediment, calculated-K_{OW}, Mabey et al. 1982)
4.17 (Lake Michigan sediment, 0.7–3.8% OC, Eadie et al. 1983)
3.36 (calculated, Sklarew & Girvin 1987)
4.09 (soil, calculated-S, Chou & Griffin 1986)
4.30, 4.12, 4.64(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 2.0 to > 10, average, Delle Site 2001)
4.82, 4.74 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: k = 0.23 μg m^{-2} d^{-1} with $t_{1/2}$ = 17 d (Baker et al. 1986);
k = 0.029 g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, k << 360 M^{-1} h^{-1} and k << 1 M^{-1} h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: 26.3% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980);
26% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980);
degraded by acclimated activated sludge with a first-order rate constant k = 0.15 d^{-1} and $t_{1/2}$ = 4.5 d (Callahan et al. 1979).
88% loss by degradation with Nocardia strain NCIB 10603, 76% loss with NCIB 10643 both within 52 d; 95% loss with NCIB 10603 and 85% loss with NCIB 10643 both within 100 d (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation: estimated k ~ 3×10^{-9} to 3×10^{-12} mL·$cell^{-1}$·h^{-1} for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ = 12 h (Paris et al. 1978); volatilization $t_{1/2}$ ~12 h at 1 m depth in 1 m^3 of water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

Groundwater:

Sediment:

Soil: $t_{1/2}$ > 50 d (Ryan et al. 1988).

Biota:

7.1.3.5 Aroclor 1248

Common Name: Aroclor 1248
Synonym:
Chemical Name:
CAS Registry No: 12672-29-6
Molecular Formula:
Average Molecular Weight: 288–299.5
Physical State: mobile oil
Distillation Range (°C):

340–375	(NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)

Chlorine Content: 48%
Density (g/cm^3):

1.44	(20°C, Brinkman & De Kock 1980)
1.40–1.41	(NAS 1979)
1.41	(Callahan et al. 1979)
1.40	(Mackay 1986; Mills et al. 1982; Metcalfe et al. 1988)

Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.10	(20°C, Nisbet & Sarofim 1972)
0.10	(Monsanto Co. 1972; selected, Hutzinger et al. 1974; Sawhney 1987)
0.043	(26°C, Hutzinger et al. 1974)
0.054	(Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983, 1986)
0.054	(NAS 1979; Callahan et al. 1979; Pal et al. 1980; Mabey et al. 1982; Mills et al. 1982; Chou & Griffin 1986)
0.060	(shake flask-nephelometry, Hollifield 1979)
0.052	(quoted, Brinkman & De Kock 1980; Erickson 1986)
0.32	(selected, Mackay 1986; Metcalfe et al. 1988)
0.056	(selected, Eisenreich 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.004	(20°C, Nisbet & Sarofim 1972)
0.066	(selected, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; quoted, Mills et al. 1982)
0.11	(20°C, extrapolated, Monsanto 1972; quoted, NAS 1979)
$\log (P_L/\text{mmHg}) = 8.40 - 3400/(T/K)$	(temp range 150–300°C, from Monsanto 1972, NAS 1979)
0.017	(Branson 1977; Kenaga & Goring 1980)
0.066	(Callahan et al. 1979; Mabey et al. 1982; Mackay et al. 1983)
0.025, 0.024	(GC-RT correlation, Foreman & Bidleman 1985)
0.0085	(selected, Eisenreich 1987)
0.023	(selected, Mackay 1986; Metcalfe et al. 1988)

Henry's Law Constant (Pa m^3/mol):

355.7	(calculated, Mackay & Leinonen 1975)
372	(Slinn et al. 1978)
364	(calculated-P/C, Mabey et al. 1982)
86.0	(calculated-P/C, Mackay et al. 1983)
44.58	(calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)
50.0	(calculated-P/C, Mackay et al. 1986)

Octanol/Water Partition Coefficient, log K_{OW}:

5.75	(Callahan et al. 1979; Kenaga & Goring 1980; Mabey et al. 1982; Chou & Griffin 1986)

6.11	(shake flask-GC, Chiou et al. 1977; quoted, Callahan et al. 1979)
6.11	(HPLC-RT correlation, Veith et al. 1979a,b; quoted, Mackay 1982; Garten & Trabalka 1983)
6.0	(quoted, Mills et al. 1982)
5.8–6.3	(quoted, Mackay et al. 1983, 1986; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
5.60	(quoted, Ryan et al. 1988)
6.10	(selected, Thomann 1989)

Bioconcentration Factor, log BCF:

4.42	(bluegill sunfish, Stalling & Meyer 1972)
4.75–4.79	(channel catfish, Mayer et al. 1977; quoted, Waid 1986)
5.08	(fathead minnow, DeFoe et al. 1978; quoted, Waid 1986)
4.85	(fathead minnow, 32-d exposure, Veith et al. 1979b)
4.86, 4.07	(fish, flowing water, static water, Kenaga & Goring 1980)
4.86	(quoted, Bysshe 1982)
3.86–4.42, 4.19	(mussel, range, average, Geyer et al. 1982)
4.86	(microorganism, calculated-K_{OW}, Mabey et al. 1982)
4.85, 4,79	(fish: quoted, calculated-K_{OW}, Mackay 1982)
4.85, 0.82, 0.72	(fish, poultry, rodents, Garten & Trabalka 1983)
4.5–5.0	(fish, selected, Mackay 1986; Metcalfe et al. 1988)
4.80, 6.08	(fathead minnow, male: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.08, 6.08	(fathead minnow, female: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.44	(sediment, calculated-K_{OW}, Mabey et al. 1982)
4.74	(soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 8.3 \times 10^{-3}$ g $m^{-2} \cdot h^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Photolysis: TiO_2 catalyzed photolytic process destroyed 80% of total PCBs in an aqueous solution and clay suspension after 4h of radiation, and 50% destroyed in sediment suspension within 6 h (Zhang et al. 1993).

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, $k << 360$ M^{-1} h^{-1} and $k << 1$ M^{-1} h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: aerobic biodegradation $t_{1/2}$ = 77.6 d without the addition of polymer chitin, $t_{1/2}$ = 38.6 d with chitin and $t_{1/2}$ = 31.9 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected form the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: estimated $k \sim 3 \times 10^{-9}$ to 3×10^{-12} mL·cell^{-1}·h^{-1} for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

log $k_2 = -1.92$ d^{-1} (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air:

Surface water: volatilization $t_{1/2} \sim 10$ h at 1 m depth in 1 m^3 water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982);

TiO_2 catalyzed photolytic process destroyed 80% of total PCBs in an aqueous solution and clay suspension after 4 h of radiation, and 50% destroyed in sediment suspension within 6 h (Zhang et al. 1993).

Groundwater:

Sediment:

Soil: $t_{1/2} > 50$ d (Ryan et al. 1988).

Biota:

7.1.3.6 Aroclor 1254

Common Name: Aroclor 1254
Synonym:
Chemical Name:
CAS Registry No: 11097-69-1
Molecular Formula:
Average Molecular Weight: 327–328.4
Physical State: viscous liquid
Distillation Range (°C):
365–390 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)
Chlorine Content: 54%
Density (g/cm^3):
1.505 (Monsanto 1972)
1.49–1.50 (65°C, NAS 1979)
1.54 (20°C Brinkman & De Kock 1980)
1.50 (Mills et al. 1982; Mackay 1986; Metcalfe et al. 1988)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.30 (Zitko 1971)
0.043 (26°C, Nelson et al. 1972)
0.050 (20°C, Nisbet & Sarofim 1972)
0.040 (Monsanto 1972; selected, Hutzinger et al. 1974; Sawhney 1987)
0.012–0.07 (Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Geyer et al. 1980; Mackay et al. 1983, 1986)
0.056 (shake flask-GC, Haque et al. 1974; quoted, Haque et al. 1980)
0.0001 (20°C, shake flask-GC/ECD, Schoor 1975)
0.045 (shake flask-GC, Lawrence & Tosine 1976)
0.070 (23°C, shake flask-GC/ECD, Griffin et al. 1978)
0.0242 (11.5°C, shake flask-GC/ECD, Dexter & Pavlou 1978)
0.012 (Brinkman & De Kock 1980; Giam et al. 1980; Pal et al. 1980; Erickson 1986)
0.010 (Kenaga & Goring 1980)
0.031 (Callahan et al. 1979; Mabey et al. 1982)
0.070 (shake flask-GC/ECD, Lee et al. 1979)
0.057 (shake flask-nephelometry, Hollifield 1979)
0.070 (23°C, Griffin & Chian 1980; quoted, Sklarew & Girvin 1987)
0.0115 (quoted, Eisenreich et al. 1981)
0.045–0.07 (quoted literature range, Westcott et al. 1981)
0.010–0.06 (quoted literature range, Mills et al. 1982)
0.042 (quoted, Chou & Griffin 1986)
0.035 (quoted, Eisenreich 1987)
0.14 (selected, Mackay 1986; Metcalfe et al. 1988)
0.043 (20°C, calculated-mole fraction, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00107 (ebulliometry, Burrows 1946)
0.00048 (20°C, Nisbet & Sarofim 1972)
0.0103 (Monsanto 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)
log (P_L/mmHg) = 8.80 – 3700/(T/K) (temp range 150–300°C, from Monsanto 1972, NAS 1979)
0.0103 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Bidleman & Christinsen 1979 Giam et al. 1980; Westcott et al. 1980)

0.024 (20°C, extrapolated, Monsanto 1974; quoted, NAS 1979)
0.0101 (quoted, Eisenreich et al. 1981)
0.004 (38°C, Average, Wingender & Williams 1984)
0.00435, 0.00424 (GC-RT correlation, Foreman & Bidleman 1985)
0.043 (selected, Mackay et al. 1986)
0.00263 (quoted, Eisenreich 1987)
6.7×10^{-3} (selected, Mackay 1986; Metcalfe et al. 1988)
0.00294 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
279.7 (calculated, Mackay & Leinonen 1975)
0.0993 (Murphy & Rzeszutko 1977; quoted, Eisenreich et al. 1983)
273 (Slinn et al. 1978)
274 (calculated-P/C, Eisenreich et al. 1981)
0.007 (Eisenreich et al. 1981a)
0.0142 (Doskey & Andren 1981; quoted, Eisenreich et al. 1983)
47.57–74.08 (calculated-P/C, Westcott et al. 1981)
16.60 (radiotracer-equilibration, Atlas et al. 1982; Atlas & Giam 1986)
21.0 (direct concn. ratio-GC/ECD, Murphy et al. 1983)
28.67 (calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)
50.0 (calculated, Mackay et al. 1986)
18.24 (20°C, selected, Murphy et al. 1987 from Burkhard et al. 1985b)
19.25 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
19.25 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 11.880 - 4099/(T/K)$, (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:—See discussion by Linkov et al. 2005.
6.03 (Hansch et al. 1973; Callahan et al. 1979; Mabey et al. 1982)
6.47 (GC-RT correlation, Veith et al. 1979b; Veith & Kosian 1983; quoted, Mackay 1982; Garten & Trabalka 1983; Zaroogian et al. 1985; Södergren 1987; Travis & Arms 1988)
6.72 (HPLC-RT correlation, Veith et al. 1979a)
4.08 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
6.0 (quoted, Mills et al. 1982)
6.79 (literature mean, Di Toro et al. 1985)
6.1–6.8 (selected, Mackay et al. 1983, 1986; Metcalfe et al. 1988)
7.17 (Rapaport & Eisenreich 1984)
6.11 (quoted, Chou & Griffin 1986)
6.50 (quoted, Thomann 1989)

Bioconcentration Factor, log BCF:
4.57 (spot fish, Hansen et al. 1971; quoted, Waid 1986)
4.85 (bluegill sunfish, Stalling & Mayer 1972)
4.75–4.79 (channel catfish, Mayer et al. 1977; quoted, Waid 1986)
5.08, 5.57, 6.08 (Mysis, sculpins, pelagic fish, Veith et al. 1977)
5.00 (fathead minnow, 32-d exposure, Veith et al. 1979b; Veith & Kosian 1983)
5.0–5.22; 4.41; 4.57 (oyster; shrimp, estuarine fish, Hansen et al. 1976; NAS 1979)
0.79, 0.78 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
4.66, 4.08 (fish, flowing water, static water, Kenaga & Goring 1980)
4.66 (quoted, Bysshe 1982)
5.12 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
5.00, 5.15 (fish: quoted, calculated-K_{OW}, Mackay 1982)
4.57 (fish, estuarine, Hansen et al. 1976; NAS 1979)
0.53, 4.70, 0.77, 0.79. 0.18, 0.98, 0.03 (cow, fish, poultry, rodents, sheep, small birds, swine, Garten & Trabalka 1983)

5.69, 5.63; 6.11, 5.76 (live bacteria, dead bacteria; live algae, dead algae, Weber, Jr. et al. 1983)
5.0 (fathead minnow, quoted, Zaroogian et al. 1985)
4.80, 4.68 (oyster, quoted, Zaroogian et al. 1985)
4.8–5.51 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
5.52 (oyster, Södergren 1987)
–1.28; –1.95; –1.77(beef; milk; vegetable, reported as biotransfer factor log B_b, log B_m, log B_v, Travis & Arms 1988)
4.95, 6.65 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
> 5.0, > 5.98 (fathead minnow, 32-d uptake: wet wt basis, lipid wt basis, Geyer et al. 2000)

Bioaccumulation Factor, log BAF:
7.21 (field data, lake trout-L/kg(lp), Thomann 1989)
6.9, 6.51, 6.67, 6.8 (field data, large-mouth bass, L/kg(lp), Thomann 1989)

Partition Coefficient, log K_P or log K_d
3.21, 3.22, 4.42, 3.56 (clay: Montmorillonite, Kaolinite, natural Blue clay, stripped Blue clay, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
4.38, 3.06, 4.73, 5.18, 4.55, 5.01, 4.50, 4.89, 4.05 (sediments: Saginaw River 1. natural, Saginaw River 1. stripped, Saginaw R. 2. natural, Saginaw River 2. NaOH ext., Saginaw River 2. benzene/MeOH ext., Saginaw River 2. stripped, Saginaw River 2. 12°C, Saginaw River 2. < 75 -m, Saignaw Bay, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
5.06, 4.95, 5.07(suspended solids: Huron River, Saginaw River1, Saginaw River 2, Weber, Jr. et al. 1983)

Sorption Partition Coefficient, log K_{OC}:
6.0 (sediment/pore water 2.0% OC of pond, Halter & Johnson 1977; selected, Di Toro et al. 1985)
5.72 (sediment, calculated-K_{OW}, Mabey et al. 1982)
5.44 (sediment/pore water 0.7–3.8% OC-Lake Michigan, Eadie et al. 1983; selected, Di Toro et al. 1985)
6.17, 6.16, 5.89 (clay: Montmorillonite 0.11% OC, natural Blue clay 1.82% OC, stripped Blue clay 0.47% OC, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
5.84, 5.04, 6.31, 6.68, 6.29, 6.19, 6.34, 7.20 (sediments: Saginaw River 1. natural 3.45% OC, Saginaw River 1. stripped 1.05% OC, Saginaw R. 2. natural 2.61% OC, Saginaw River 2. NaOH ext. 1.98% OC, Saginaw River 2. benzene/MeOH ext. 1.84% OC, Saginaw River 2. stripped 0.67% OC, Saginaw River 2. < 75 μm 3.51% OC, Saignaw Bay 0.07% OC, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
6.10, 5.97, 6.15 (suspended solids: Huron River 9.25% OC, Saginaw River 1. 9.48% OC, Saginaw River 2. 8.30% OC, batch equilibrium, Weber, Jr. et al. 1983)
6.65 (suspended solids/subsurface water, 56% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.88 (sediment/pore water, 0.7% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.61 (sediment/pore water, 1.7% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
4.82 (sediment/pore water, 3.8% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
6.62 (calculated, Sklarew & Girvin 1987)
4.81 (soil, calculated-S, Chou & Griffin 1986)
6.02 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:
Volatilization/Evaporation: volatilization rate k ~ 2×10^{-6} g cm^{-2} d^{-1} at 26°C and k = 8.6×10^{-5} g cm^{-2} d^{-1} at 60°C (Haque et al. 1974);
k = 0.10 μg m^{-2} d^{-1} with $t_{½}$ = 28 d (Baker et al. 1985);
k = 2.7×10^{-3} g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis: not environmentally significant.

Oxidation: calculated rate constant for singlet oxygen, k << 360 M^{-1} h^{-1} and, k << 1 M^{-1} h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: no reduction of concentration in the spilled transformer fluid contaminant of Aroclor was detected over a two-year period (Moein et al. 1976; quoted, Pal et al. 1980).
15.2% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972);
19% degraded by activated sludge for 48-h exposure (Callahan et al. 1979);
biodegradation with a first-order k = 0.1 d^{-1} by acclimated activated sludge and $t_{1/2}$ = 7.0 d (Callahan et al. 1979);
aerobic biodegradation $t_{1/2}$ = 81.9 d without the addition of polymer chitin, $t_{1/2}$ = 36.4 d with chitin and $t_{1/2}$ = 35.5 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: estimated k ~ 3×10^{-9} to 3×10^{-12} mL·cell^{-1}·h^{-1} for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.023 d^{-1} (0 to 1 d), k_2 = 0.086 d^{-1} (1 to 2 d), and k_2 = 0.0899 d^{-1} (2 to 6 d) with a biological $t_{1/2}$ = 5.5 d (mosquito larvae, Gooch & Hamdy 1982; selected, Waid 1986)
k_2 = 0.131 d^{-1}, 0.137 d^{-1} with biological $t_{1/2}$ = 4.7 d (guppies, Gooch & Hamdy 1982; quoted, Waid 1986)
k_2 = 0.102 d^{-1} (first day), k_2 = 0.057 d^{-1} (thereafter) with a biological $t_{1/2}$ = 6.1 d (cichlids, Gooch & Hamdy 1982; quoted, Waid 1986)

Half-Lives in the Environment:

Air:

Surface water: volatilization $t_{1/2}$ ~ 10 h from 1 meter depth in 1 m^3 water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

Groundwater:

Sediment:

Soil: volatilization $t_{1/2}$ ~ 15 d from an Ottawa sand (Haque et al. 1974; quoted, Pal et al. 1980);
$t_{1/2}$ > 50 d in soil (Ryan et al. 1988).

Biota: $t_{1/2}$ < 12 d in plant surface (Pal et al. 1980);
$t_{1/2}$ = 3.3 d in guppies, and $t_{1/2}$ = 5.1 d cichlids (Gooch & Hamdy 1982; quoted, Waid 1986).

7.1.3.7 Aroclor 1260

Common Name: Aroclor 1260
Synonym:
Chemical Name:
CAS Registry No: 11096-82-5
Molecular Formula:
Average Molecular Weight: 372–375.7
Physical State: sticky resin
Distillation Range (°C):
385–420 (NAS 1979; Brinkman & De Kock 1980)
Chlorine Content: 60%
Density (g/cm^3):
1.62 (20°C, Brinkman & De Kock 1980)
1.55–1.56 (90°C, NAS 1979)
1.58 (Callahan et al. 1979; Mills et al. 1982)
1.60 (Mackay 1986; Metcalfe et al. 1988)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.025 (Monsanto 1972)
0.025 (20°C, Nisbet & Sarofim 1972)
0.0027 (Mackay & Wolkoff 1973; quoted, Callahan et al. 1979; Geyer et al. 1980; Pal et al. 1980; Mabey et al. 1982; Mills et al. 1982; Richardson et al. 1983; Chou & Griffin 1986)
0.080 (shake flask-nephelometry, Hollifield 1979)
0.003 (quoted, Brinkman & De Kock 1980; Mackay et al. 1983; Eisenreich 1987)
0.0144 (20°C, calculated-mole fraction, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C or indicated and reported temperature dependence equations):
2.67×10^{-5} (38°C, Nisbet & Sarofim 1972)
0.0054 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983)
0.012 (20°C, extrapolated, Monsanto 1972; NAS 1979)
$\log (P_L/\text{mmHg}) = 8.50 - 3700/(T/K)$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)
0.0054 (Callahan et al. 1979; Mabey et al. 1982; Richardson et al. 1983)
0.0053 (Pal et al. 1980; Mills et al. 1982)
0.0004 (38°C, average, Wingender & Williams 1984)
0.00183, 0.00162 (GC-RT, Foreman & Bidleman 1985)
0.003 (quoted, Erickson 1986)
0.00064 (Mackay 1986; Metcalfe et al. 1988)
0.000284 (quoted, Eisenreich 1987)
0.000841 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m^3/mol):
722.4 (calculated, Mackay & Leinonen 1975)
718 (Slinn et al. 1978)
719 (quoted, Mills et al. 1982)
88.0 (suggested, Mackay et al. 1983)
72.24 (16°C, calculated-P/C, Richardson et al. 1983)
34.04 (calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)
21.27 (20°C, quoted, Murphy et al. 1987 from Burkhard et al. 1985b)

17.23	(20°C, equilibrium concn. ratio, Murphy et al. 1987)
17.23	(20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 11.848 - 4104/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

7.14	(Chiou et al. 1977)
6.11	(Chiou et al. 1977; Callahan et al. 1979; quoted, Ryan et al. 1988)
7.15	(Callahan et al. 1979; Mabey et al. 1982)
6.91	(GC-RT correlation, Veith et al. 1979a; Veith & Kosian 1983; quoted, Mackay 1982; Geyer et al. 1987)
4.34	(Pal et al. 1980)
> 6.0	(quoted, Mills et al. 1982)
6.30–7.50	(quoted, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
6.61	(calculated-S, Chou & Griffin 1986)
6.90	(quoted, Thomann 1989)

Bioconcentration Factor, log BCF:

5.43	(fathead minnows, DeFoe et al. 1978; quoted, Waid 1986)
5.29	(fathead minnow, 32-d exposure, Veith et al. 1979a; Veith & Kosian 1983)
0.672	(adipose tissue of male albino rats, Geyer et al. 1980)
5.29, 5.59	(fish: quoted, calculated-K_{OW}, Mackay 1982)
6.11	(microorganism, calculated-K_{OW}, Mabey et al. 1982)
5.0–6.20	(fish, quoted, Mackay 1986; Metcalfe et al. 1988)
2.28–2.50	(human fat of lipid basis, calculated-K_{OW}, Geyer et al. 1987)
2.11–2.36	(human fat of wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
4.38	(*Rhabdosargus holubi*, De Kock & Lord 1988)
4.80, 6.72	(oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.22, 6.50	(fathead minnow, male, 250-d uptake: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.43, 6.53	(fathead minnow, female, 250-d uptake, wet wt basis, lipid wt basis, Geyer et al. 2000)
2.24, 2.40	(human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.83	(sediment, calculated-K_{OW}, Mabey et al. 1982)
5.54	(soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: estimated evaporation rate from liquid surfaces at 100°C to be 0.009 mg/cm^2·h (Hutzinger et al. 1974);
$t_{½}$ ~ 7.53 h of evaporation from water depth of 1 m (Mackay & Leinonen 1975)
rate of evaporation $k = 2.9 \times 10^{-4}$ g m^{-2}·h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, $k << 360$ M^{-1}·h^{-1} and $k << 1$ M^{-1}·h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: no degradation over a 12-week period in natural water samples (Oloffs et al. 1972; quoted, Pal et al. 1980).

Biotransformation: $k \sim 3 \times 10^{-9}$ to 3×10^{-12} mL·cell^{-1}·h^{-1}, transformation for bacteria in water (Mabey et al. 1982)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 332$ d^{-1}; $k_2 = 0.014$ d^{-1} (*Rhabdosargus holubi*, De Kock & Lord 1988)
$\log k_2 = -2.40$ d^{-1} (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air:
Surface water: volatilization $t_{½}$ ~ 10 h at 1 m depth of 1 m^3 of water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).
River water: volatilization $t_{½}$ ~ 52 d (Oloffs et al. 1972; selected, Pal et al. 1980).
Sediment:
Soil:
Biota: $t_{½}$ = 50 d in *Rhabdosargus holubi* (De Kock & Lord 1988).

7.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 7.2.1
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V_M (cm^3/mol)
0	Biphenyl	92-52-4	154.207	68.93	256.1	0.371	184.6
1	2-	2051-60-7	188.652	34	274	0.816	205.5
2	3-	2051-61-8	188.652	16	284.5	1	205.5
3	4-	2051-62-9	188.652	78.8	292.9	0.297	205.5
4	2,2′-	13029-08-8	223.098	60.5		0.448	226.4
5	2,3-	16605-91-7	223.098	28		0.934	226.4
6	2,3′	25569–80–6	223.098				226.4
7	2,4-	33284-50-3	223.098	24.4		1	226.4
8	2,4′-	34883-43-7	223.098	43		0.666	226.4
9	2,5-	34883-39-1	223.098	22–23		1	226.4
10	2,6-	33146-45-1	223.098	35.5		0.789	226.4
11	3,3′-	2050-67-1	223.098	29	320	0.914	226.4
12	3,4-	2974-92-7	223.098	49	195–200	0.581	226.4
13	3,4′-	2974–90–5	223.098				226.4
14	3,5-	34883-41-5	223.098	31		0.873	226.4
15	4,4′-	2050-68-2	223.098	149.3	317	0.0603	226.4
16	2,2′,3-	38444-78-9	257.543	28		0.934	247.3
17	2,2′,4-	37680–66–3	257.543				247.3
18	2,2′,5-	37680-65-2	257.543	44		0.651	247.3
19	2,2′,6-	38444–73–4	257.543				247.3
20	2,3,3′-	38444-84-7	257.543				247.3
21	2,3,4-	55702-46-0	257.543	102		0.176	247.3
22	2,3,4′-	38444–85–8	257.543	73		0.338	247.3
23	2,3,5-	55720–44–0	257.543	41		0.697	247.3
24	2,3,6-	55702–45–9	257.543	49		0.581	247.3
25	2,3′,4-	55712–37–3	257.543				247.3
26	2,3′,5-	38444–81–4	257.543	40.5		0.705	247.3
27	2,3′,6-	38444–76–7	257.543				247.3
28	2,4,4′-	7012-37-5	257.543	57		0.485	247.3
29	2,4,5-	15862-07-4	257.543	78.5		0.299	247.3

(Continued)

TABLE 7.2.1 *(Continued)*
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V_M (cm^3/mol)
30	2,4,6-	35693-92-6	257.543	62.5		0.429	247.3
31	2,4′,5-	16606–02–3	257.543	67		0.387	247.3
32	2,4′,6-	38444–77–8	257.543				247.3
33	2,3′,4′-	38444-86-9	257.543	60		0.454	247.3
34	2,3′,5′-	37680–68–5	257.543	58		0.474	247.3
35	3,3′,4-	37680-69-6	257.543	87		0.246	247.3
36	3,3′,5-	38444–87–0	257.543				247.3
37	3,4,4′-	38444-90-5	257.543	87		0.246	247.3
38	3,4,5-	53555–66–1	257.543				247.3
39	3,4′,5-	38444–88–1	257.543	88		0.241	247.3
40	2,2′,3,3′-	38444-93-8	291.988	121		0.114	268.2
41	2,2′,3,4-	52663–59–9	291.988				268.2
42	2,2′,3,4′-	36559–22–5	291.988	69		0.370	268.2
43	2,2′,3,5-	70362–46–8	291.988				268.2
44	2,2′,3,5′-	41464-39-5	291.988	47		0.608	268.2
45	2,2′,3,6-	70362–45–7	291.988				268.2
46	2,2′,3,6′-	41464–47–5	291.988				268.2
47	2,2′,4,4′-	2437-79-8	291.988	83		0.270	268.2
48	2,2′,4,5-	70362–47–9	291.988	65.9		0.397	268.2
49	2,2′,4, 5′-	41464-40-8	291.988	66.5		0.392	268.2
50	2,2′,4,6-	62796-65-8	291.988				268.2
51	2,2′,4,6′-	68194-04-7	291.988	66		0.396	268.2
52	2,2′,5,5′-	35693-99-3	291.988	87		0.246	268.2
53	2,2′,5,6′-	41464-41-9	291.988	104		0.168	268.2
54	2,2′,6,6′-	15968-05-5	291.988	198		0.0201	268.2
55	2,3,3′,4-	74338–24–2	291.988				268.2
56	2,3,3′,4′-	41464–43–1	291.988				268.2
57	2,3,3′,5-	70424–67–8	291.988				268.2
58	2,3,3′,5′-	41464–49–7	291.988				268.2
59	2,3,3′,6-	74472–33–6	291.988				268.2
60	2,3,4,4′-	33025-41-1	291.988	142		0.0711	268.2
61	2,3,4,5-	33284-53-6	291.988	92.2		0.219	268.2
62	2,3,4,6-	54230–23–7	291.988				268.2

63	2,3,4′,5-	74472–34–7	291.988			268.2
64	2,3,4′,6-	52663–58–8	291.988			268.2
65	2,3,5,6-	33284-54-7	291.988	79	0.295	268.2
66	2,3′,4,4′-	32598-10-0	291.988	124	0.107	268.2
67	2,3′,4,5-	73575–53–8	291.988			268.2
68	2,3′,4,5′-	73575–52–7	291.988			268.2
69	2,3′,4,6-	60233–24–1	291.988			268.2
70	2,3′,4′,5-	32598-11-1	291.988	104	0.168	268.2
71	2,3′,4′,6-	41464–46–4	291.988			268.2
72	2,4′,5,5′-	41464–42–0	291.988			268.2
73	2,3′,5′,6-	74338–23–1	291.988			268.2
74	2,4,4′,5-	32690–93–0	291.988	125	0.104	268.2
75	2,4,4′,6-	32598-12-2	291.988			268.2
76	2,3′,4′,5′-	70362–48–0	291.988			268.2
77	3,3′,4,4′-	32598-13-3	291.988	180	0.0301	268.2
78	3,3′,4,5-	70362–49–1	291.988			268.2
79	3,3′,4,5′-	41464–48–6	291.988			268.2
80	3,3′,5,5′-	33284-52-5	291.988	164	0.0433	268.2
81	3,4,4′,5-	70362–50–4	291.988			268.2
82	2,2′,3,3′,4-	52663–62–4	326.433			289.1
83	2,2′,3,3′,5-	60145-20-2	326.433	65	0.405	289.1
84	2,2′,3,3′,6-	52663–60–2	326.433			289.1
85	2,2′,3,4,4′-	65510–45–4	326.433			289.1
86	2,2′,3,4,5-	55312-69-1	326.433	100	0.184	289.1
87	2,2′,3,4,5′-	38380-02-8	326.433	114	0.134	289.1
88	2,2′,3,4,6-	55215-17-3	326.433	100	0.184	289.1
89	2,2′,3,4,6′-	73575–57–2	326.433			289.1
90	2,2′,3,4′,5-	68194–07–0	326.433			289.1
91	2,2′,3,4′,6-	58194–05–8	326.433			289.1
92	2,2′,3,5,5′-	52663–61–3	326.433			289.1
93	2,2′,3,5,6-	73575–56–1	326.433			289.1
94	2,2′,3,5,6′-	73575–55–0	326.433			289.1
95	2,2′3,5,6-	38379-99-6	326.433	100	0.184	289.1
96	2,2′,3,6,6′-	73575–54–9	326.433			289.1
97	2,2′,3,4′,5′-	41464–51–1	326.433	82	0.276	289.1
98	2,2′,3,4′,6′-	60233–25–2	326.433			289.1
99	2,2′,4,4′,5-	38380-01-7	326.433			289.1

(Continued)

TABLE 7.2.1 (*Continued*)
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V_M (cm^3/mol)
100	2,2′4,4′,6-	39485-83-1	326.433				289.1
101	2,2′,4,5,5′-	37680-73-2	326.433	78.5		0.299	289.1
102	2,2′,4,5,6′-	68194–06–9	326.433				289.1
103	2,2′,4,5′,6-	60145–21–3	326.433				289.1
104	2,2′,4,6,6′-	56558-16-8	326.433	85		0.258	289.1
105	2,3,3′,4,4′-	32598-14-4	326.433	105		0.164	289.1
106	2,3,3′,4,5-	70424–69–0	326.433				289.1
107	2,3,3′,4′,5-	70424–68–9	326.433				289.1
108	2,3,3′,4,5′-	70362–41–3	326.433				289.1
109	2,3,3′,4,6-	74472–35–8	326.433				289.1
110	2,3,3′,4′,6-	38380-03-9	326.433				289.1
111	2,3,3′,5,5′-	39635–32–0	326.433				289.1
112	2,3,3′,5,6-	74472–36–9	326.433				289.1
113	2,3,3′,5′,6-	68194–10–5	326.433				289.1
114	2,3,4,4′,5-	74472–37–0	326.433	99		0.188	289.1
115	2,3,4,4′,6-	74472–38–1	326.433				289.1
116	2,3,4,5,6-	18259-05-7	326.433	123.5		0.108	289.1
117	2,3,4′,5,6-	68194–11–6	326.433				289.1
118	2,3′,4,4′,5-	31508-00-6	326.433	107		0.157	289.1
119	2,3′,4,4′,6-	56558–17–9	326.433				289.1
120	2,3′,4,5,5′-	68194–12–7	326.433	77		0.309	289.1
121	2,3′,4,5′,6-	56558–18–0	326.433				289.1
122	2,3,3′,4′,5′-	76842–07–4	326.433				289.1
123	2,3′,4,4′,5′-	65510–44–3	326.433				289.1
124	2,3′,4′,5,5′-	70424-70-3	326.433				289.1
125	2,3′,4′,5′,6-	74472–39–2	326.433				289.1
126	3,3′,4,4′,5-	57465–28–8	326.433	106		0.160	289.1
127	3,3′,4,5,5′-	39635–33–1	326.433				289.1
128	2,2′,3,3′,4,4′-	38380-07-3	360.878	151		0.058	310.0
129	2,2′,3,3′4,5-	55215-18-4	360.878	85		0.258	310.0
130	2,2′,3,3′,4,5′-	52663–66–8	360.878				310.0
131	2,2′,3,3′,4,6-	61798–70–7	360.878				310.0
132	2,2′,3,3′,4,6′-	38380–05–1	360.878				310.0

133	2,2′,3,3′,5,5′-	35694–04–3	360.878	129	0.0954	310.0
134	2,2′,3,3′,5,6-	52704-70-8	360.878	100	0.184	310.0
135	2,2′,3,3′,5,6′-	52744–13–5	360.878			310.0
136	2,2′,3,3′,6,6′-	38411-22-2	360.878	114.2	0.133	310.0
137	2,2′,3,4,4′,5-	35694–06–5	360.878	78	0.302	310.0
138	2,2′,3,4,4′,5′-	35065-28-2	360.878	80	0.289	310.0
139	2,2′,3,4,4′,6-	56030–56–9	360.878			310.0
140	2,2′,3,4,4′,6′-	59291–64–4	360.878			310.0
141	2,2,3,4,5,5′-	52712–04–6	360.878	85	0.258	310.0
142	2,2′,3,4,5,6-	41411–61–4	360.878	136	0.0815	310.0
143	2,2′,3,4,5,6′-	68194–15–0	360.878			310.0
144	2,2′,3,4,5′,6-	68194–14–9	360.878			310.0
145	2,2′,3,4,6,6′-	74472–40–5	360.878			310.0
146	2,2′,3,4′,5,5′-	51908–16–8	360.878			310.0
147	2,2′,3,4′,5,6-	68194–13–8	360.878			310.0
148	2,2′,3,4′,5,6′-	74472–42–7	360.878			310.0
149	2,2′,3,4′,5′,6-	38380-04-0	360.878	oil	1	310.0
150	2,2′,3,4′,6,6′-	68194–08–1	360.878			310.0
151	2,2′,3,5,5′,6-	52663–63–5	360.878	101	0.180	310.0
152	2,2′,3,5,6,6′-	68194–09–2	360.878			310.0
153	2,2′,4,4′,5,5′-	35065-27-1	360.878	103.5	0.170	310.0
154	2,2′,4,4′,5,6′-	60145–22–4	360.878	oil	1	310.0
155	2,2′,4,4′,6,6′-	33979-03-2	360.878	112.5	0.139	310.0
156	2,3,3′,4,4′,5-	38380-08-4	360.878	127	0.100	310.0
157	2,3,3′,4,4′,5′-	69782–90–7	360.878			310.0
158	2,3,3′,4,4′,6	74472–42–7	360.878	107	0.157	310.0
159	2,3,3′,4,5,5′-	39635–35–3	360.878			310.0
160	2,3,3′,4,5,6-	41411–62–5	360.878	99	0.188	310.0
161	2,3,3′,4,5′,6-	74472–43–8	360.878			310.0
162	2,3,3′,4′,5,5′-	39635–34–2	360.878			310.0
163	2,3,3′,4′,5,6-	74472–44–9	360.878			310.0
164	2,3,3′,4′,5′,6-	74472–45–0	360.878			310.0
165	2,3,3′,5,5′,6-	74472–46–1	360.878			310.0
166	2,3,4,4′,5,6-	41411–63–6	360.878	163	0.0433	310.0
167	2,3′,4,4′,5,5′-	52663–72–6	360.878			310.0
168	2,3′,4,4′,5′,6-	59291–65–5	360.878	110–111	0.145	310.0
169	3,3′4,4′,5,5′-	32774-16-6	360.878	202	0.0183	310.0
170	2,2′,3,3′,4,4′,5-	35065-30-6	395.323	135	0.0833	330.9

(Continued)

TABLE 7.2.1
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. ºC	b.p. ºC	Fugacity ratio, F at 25°C*	Le Bas molar volume, V_M (cm^3/mol)
171	2,2′,3,3′,4,4′,6-	52663-71-5	395.323	117.5		0.124	330.9
172	2,2′,3,3′,4,5,5′-	52663–74–8	395.323				330.9
173	2,2′,3,3′,4,5,6-	68194–16–1	395.323				330.9
174	2,2′,3,3′,4,5,6′-	38411–25–5	395.323	130.6		0.0920	330.9
175	2,2′,3,3′,4,5′,6-	40186–70–7	395.323				330.9
176	2,2′,3,3′,4,5,6′-	52663–65–7	395.323				330.9
177	2,2′,3,3′,4′,5,6-	52663–70–4	395.323				330.9
178	2,2′,3,3′,5,5′,6-	52663–67–9	395.323				330.9
179	2,2′,3,3′,5,6,6′-	52663–64–6	395.323				330.9
180	2,2′,3,4,4′,5,5′-	35065-29-3	395.323	110		0.147	330.9
181	2,2′,3,4,4′,5,6-	74472–47–2	395.323				330.9
182	2,2′,3,4,4′,5,6′-	60145–23–5	395.323	152		0.0567	330.9
183	2,2′,3,4,4′,5′,6-	52663–69–1	395.323	83		0.270	330.9
184	2,2′,3,4,4′,6,6′-	74472–48–3	395.323				330.9
185	2,2′,3,4,5,5′,6-	52712-05-7	395.323	149		0.0607	330.9
186	2,2′,3,4,5,6,6′-	74472–49–4	395.323				330.9
187	2,2′,3,4′,5,5′,6-	52663-68-0	395.323	149		0.0607	330.9
188	2,2′,3,4′,5,6,6′-	74487–85–7	395.323				330.9
189	2,3,3′,4,4′,5,5′-	39635–31–9	395.323	170		0.0378	330.9
190	2,3,3′,4,4′,5,6-	41411–64–7	395.323	117		0.125	330.9
191	2,3,3′,4,4′,5′,6-	74472–50–7	395.323				330.9
192	2,3,3′,4,5,5′,6-	74472–51–8	395.323				330.9
193	2,3,3′,4′,5,5′,6-	69782–91–8	395.323				330.9
194	2,2′,3,3′,4,4′,5,5′-	35694-08-7	429.768	159		0.0484	351.8
195	2,2′,3,3′,4,4′,5,6-	52663–78–2	429.768				351.8
196	2,2′,3,3′,4,4′,5,6′-	42740–50–1	429.768				351.8
197	2,2′,3,3′,4,4′,6,6′-	33091–17–7	429.768	132		0.0892	351.8
198	2,2′,3,3′,4,5,5′,6-	68194–17–2	429.768				351.8
199	2,2′,3,3′,4,5,5′,6′-	52663–75–9	429.768				1.759
200	2,2′,3,3′,4,5,6,6'-	52663–73–7	429.768				351.8
201	2,2′,3,3′,4,5′,6,6′-	40186–71–8	429.768				351.8

202	2,2′,3,3′,5,5′,6,6′-	2136-99-4	429.768	161		0.0463	351.8
203	2,2′,3,4,4′,5,5′,6-	52663–76–0	429.768				351.8
204	2,2′,3,4,4′,5,6,6′-	74472–52–9	429.768				351.8
205	2,3,3′,4,4′,5,5′,6-	74472–53–0	429.768				351.8
206	2,2′,3,3′,4,4′,5,5′,6-	40186-72-9	464.213	206		0.0168	372.7
207	2,2′,3,3′,4,4′,5,6,6′-	52663-79-3	464.213				372.7
208	2,2′,3,3′,4,5,5′,6,6′-	52663-77-1	464.213	180.5		0.0298	372.7
209	2,2′,3,3′,4,4′,5,5′,6,6′-	2051-24-3	498.658	309		0.00164	393.6

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 7.2.2
Summary of selected physical-chemical properties of some PCB congeners at 25 °C

		Selected properties:						
		Vapor pressure		Solubility				
IUPAC no.	Congener	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mmol/m³)	C_L/(mmol/m³)	log K_{OW}	Henry's law const. H/(Pa·m³/mol) calculated P/C
0	Biphenyl	1.3	3.50	7	45.39	122.4	3.9	28.64
1	2-	2.04	2.5	5.5	29.15	35.73	4.3	69.97
2	3-	1	1	2.5	13.25	13.24	4.6	75.46
3	4-	0.271	0.91	1.2	6.36	21.42	4.5	42.60
4	2,2′-	0.265	0.59	1	4.482	10.00	4.9	59.12
7	2,4-	0.254	0.254	1.25	5.603	5.603	5.0	45.33
8	2,4′-			1	4.482	6.730	5.1	
9	2,5-	0.18	0.18	2	8.960	8.960	5.1	20.08
10	2,6-			1.4	6.275	7.840	5.0	
11	3,3′-	0.027	0.030	0.354	1.587	1.736	5.3	17.02
12	3,4-			0.008	0.0358	0.0617		
14	3,5-	0.105	0.120					
15	4,4′-	0.0048	0.080	0.06	0.269	4.460	5.3	17.84
18	2,2′,5-	0.143	0.220	0.4	1.553	2.386	5.6	92.07
26	2,3′,5-			0.251	0.975	1.382		
28	2,4,4′-			0.16	0.621	1.281	5.8	
29	2,4,5-	0.132	0.441	0.14	0.544	1.818	5.6	242.8
30	2,4,6-	0.0384	0.090	0.2	0.777	1.810	5.5	49.45
33	2,3′,4′-	0.0136	0.003	0.08	0.311	0.684	5.8	43.78
37	3,4,4′-			0.015	0.0582	0.237	5.9	
40	2,2′,3,3v-	0.00225	0.0197	0.03	0.103	0.901	5.6	21.90
44	2,2′,3,5′-			0.1	0.342	0.563	6.0	
47	2,2′,4,4′-	0.0054	0.02	0.09	0.308	1.142	5.9	17.52
49	2,2′,4,5′-			0.016	0.0548	0.149	6.1	
52	2,2′,5,5′-	0.0049	0.02	0.03	0.103	0.418	6.1	47.69
53	2,2′,5,6′-						5.5	
54	2,2′,6,6′-						5.48	
60	2,3,4,4′-						6.31	
61	2,3,4,5-			0.02	0.0685	0.313	5.9	
65	2,3,5,6-						5.94	
66	2,3′,4,4′-			0.04	0.137	1.280	5.8	

75	2,4,4′,6-			0.091	0.312		6.21	
77	3,3′,4,4′-	5.88×10^{-5}	0.002	0.001	0.00342	0.114	6.5	17.16
80	3,3′,5,5′-			0.0012	0.0041	0.0949		
86	2,2′,3,4,5-	0.00927	0.0504	0.02	0.0613	0.333	6.2	151.3
87	2,2′,3,4,5′-	0.000304	0.00227	0.004	0.0123	0.0914	6.5	24.81
88	2,2′,3,4,6-			0.012	0.0368	0.200	6.5	
101	2,2′,4,5,5′-	0.00109	0.00364	0.01	0.0306	0.102	6.4	35.58
104	2,2′,4,6,6′-		0.00434	0.0156	0.0478	0.185		23.43
105	2,3,3′,4,4′-						6.0	
110	2,3,3′,4′,6-			0.004	0.0123		6.3	
116	2,3,4,5,6-			0.008	0.0245	0.227	6.3	
128	2,2′,3,3′,4,4′-	1.98×10^{-5}	0.00034	0.0006	0.00166	0.0286	7.0	11.91
129	2,2′,3,3′4,5-			0.0006	0.00166	0.0064	7.3	
134	2,2′,3,3′,5,6-			0.0004	0.00111	0.0060	7.3	
136	2,2′,3,3′,6,6′-			0.0008	0.00222	0.0167	6.7	
153	2,2′,4,4′,5,5′-	0.000119	0.0007	0.001	0.00277	0.0163	6.9	42.94
155	2,2′,4,4′,6,6′-	0.00048	0.00345	0.002	0.00554	0.0399	7.0	86.62
171	2,2′,3,3′,4,4′,6-	2.73×10^{-5}	0.00022	0.002	0.00506	0.0408	6.7	5.396
185	2,2′,3,4,5,5′,6-			0.00045	0.00114	0.0188	7.0	
194	2,2′,3,3′,4,4′,5,5′-			0.0002	0.00047	0.00962	7.4	
202	2,2′,3,3′,5,5′,6,6′-	2.66×10^{-5}	0.0006	0.0003	0.0007	0.0158	7.1	38.11
206	2,2′,3,3′,4,4′,5,5′,6-	1.96×10^{-7}	1.17×10^{-5}	0.00011	0.000237	0.0141	7.2	0.8271
207	2,2′,3,3′,4,4′,5,6,6′-						7.52	
208	2,2′,3,3′,4,5,5′,6,6′-			1.8×10^{-5}	3.88×10^{-5}	0.00130	8.16	
209	2,2′,3,3′,4,4′,5,5′,6,6′-	5.02×10^{-8}	3.06×10^{-5}	1.0×10^{-6}	2.00×10^{-6}	0.0122	8.26	25.03

TABLE 7.2.3
Summary of physical properties of PCB isomer groups and Aroclor mixtures

PCB isomer group	CAS no.	Molecular weight, MW g/mol	Cl no.	m.p. °C	Fugacity ratio, F range at 25°C	Le Bas molar volume, V_M (cm^3/mol)
Biphenyl	92-52-4	154.2	0	71	0.352	184.6
Monochloro-	27323-18-8	188.7	1	25.1–78	0.299–1.0	205.5
Dichloro-	25512-42-9	223.1	2	24.4–149	0.0594–1.0	226.4
Trichloro-	25323-68-6	257.5	3	28.1–102	0.173–0.932	247.3
Tetrachloro-	26914-33-0	292.0	4	47–164	0.042–0.606	268.2
Pentachloro-	25429-29-2	326.4	5	76.5–123	0.107–0.310	289.1
Hexachloro-	26601-64-9	360.9	6	70–201	0.0182–0.359	310
Heptachloro-	28655-71-2	395.3	7	109–162	0.0596–0.148	330.9
Octachloro-	31472-83-0	429.8	8	132–161	0.0452–0.0874474	351.8
Nonachloro-	53742-07-7	464.2	9	205–206	0.0163–0.0276	372.7
Decachloro-	2051-24-3	498.7	10	305	0.00167	393.6

Aroclor mixture	CAS no.	Molecular weight, MW g/mol	% Cl	No. of Cl/molecule	Fugacity ratio, F at 25°C	Density g/cm^3 at 25°C	Distillation range °C
Aroclor 1016	12674-11-2	257	41	3	1.0	1.33	323–356
Aroclor 1221	111-042-82	192	20.5–21.5	1.15	1.0	1.15	275–320
Aroclor 1232	111-411-65	221	31.4–32.5	2.04	1.0	1.24	290–325
Aroclor 1242	534-692-19	261	42	3.1	1.0	1.35	325–366
Aroclor 1248	126-722-96	288	48	3.9	1.0	1.41	340–375
Aroclor 1254	110-976-91	327	54	4.96	1.0	1.5	365–390
Aroclor 1260	110-968-25	372	60	6.3	1.0	1.58	385–420

TABLE 7.2.4
Summary of selected physical-chemical properties of PCB isomer groups and Aroclor mixtures at 20–25°C

PCB isomer group	Aqueous solubility range			Vapor pressure range		Henry's law const. H/(Pa·m³/mol) calculated P/C	log K_{OW} range
	$S/(g/m^3)$	$C_S/(mmol/m^3)$	$C_L/(mmol/m^3)$	P_S/Pa	P_L/Pa		
Biphenyl	7.0	45.39	129.7	1.30	3.69	28.64	3.90
Monochloro-	1.21–5.50	6.36-29.15	1 13.24-35.66	0.271-2.04	0.9-2.5	42.56-75.55	4.3-4.60
Dichloro-	0.060–2.0	0.269-8.96	4.56-10.14	0.0048-0.279	0.008-0.60	17.0-92.21	4.9-5.30
Trichloro-	0.015–0.40	0.0582-1.55	0.24-2.39	0.0136-0.143	0.003-0.22	24.29-92.21	5.5-5.90
Tetrachloro-	0.0043–0.010	0.0147-0.342	0.133-1.30	0.000059-.0054	0.002	1.72-47.59	5.6-6.50
Pentachloro-	0.004–0.020	0.0123-0.0613	0.093-0.337	0.000304-0.0093	0.0023-0.051	24.8-151.4	6.2-6.50
Hexachloro-	0.0004–0.0007	0.0011-0.002	0.0061-0.0286	0.000020-0.00159	0.0007- 0.012	11.9-818	6.7-7.30
Heptachloro-	0.000045–0.0002	0.00114-0.0051	0.0191-0.046	0.0000273	0.00025	5.40	6.7-7.0
Octachloro-	0.0002–0.0003	0.00047-0.0007	0.0098-0.0158	0.0000266	0.0006	38.08	7.10
Nonachloro-	0.00018–0.0012	0.000038-0.00024	0.00141-0.0146	-	-	-	7.2-8.16
Decachloro-	0.000761	0.0000024	0.0144	0.00000005	0.00003	20.84	8.26

Aroclor mixture	Aqueous solubility range		Vapor pressure range	Henry's law const. H/(Pa·m³/mol) calculated P/C	log K_{OW} range
	$S/(g/m^3)$	$C_L/(mmol/m^3)$	P_L/Pa		
Aroclor 1016	0.22-0.84	0.856-0.216	0.06-0.2	70-900	4.4-5.8
Aroclor 1221	0.59-5.0	0.307-26.0	0.89-2.0	34-450	4.1-4.7
Aroclor 1232	1.45	6.56-2.0	0.54	82-270	4.5-5.2
Aroclor 1242	0.1-0.75	0.383-2.87	0.05-0.13	45-130	4.5-5.8
Aroclor 1248	0.1-0.5	0.347-1.74	0.0085-0.11	5-300	5.8-6.3
Aroclor 1254	0.01-0.30	0.306-0.92	0.008-0.02	20-260	6.1-6.8*
Aroclor 1260	0.003-0.08	0.00806-0.215	0.0002-0.012	20-60	6.3-6.8*

* See discussion by Linkov et al. 2005.

TABLE 7.2.5
Suggested half-life classes of polychlorinated biphenyls (PCBs) in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Biphenyl	3	4	5	6
Monochloro-	4	7	8	8
Dichloro-	4	7	8	8
Trichloro-	5	8	9	9
Tetrachloro-	6	9	9	9
Pentachloro-	6	9	9	9
Hexachloro-	7	9	9	9
Heptachloro-	7	9	9	9
Octachloro-	8	9	9	9
Nonachloro-	8	9	9	9
Decachloro-	9	9	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

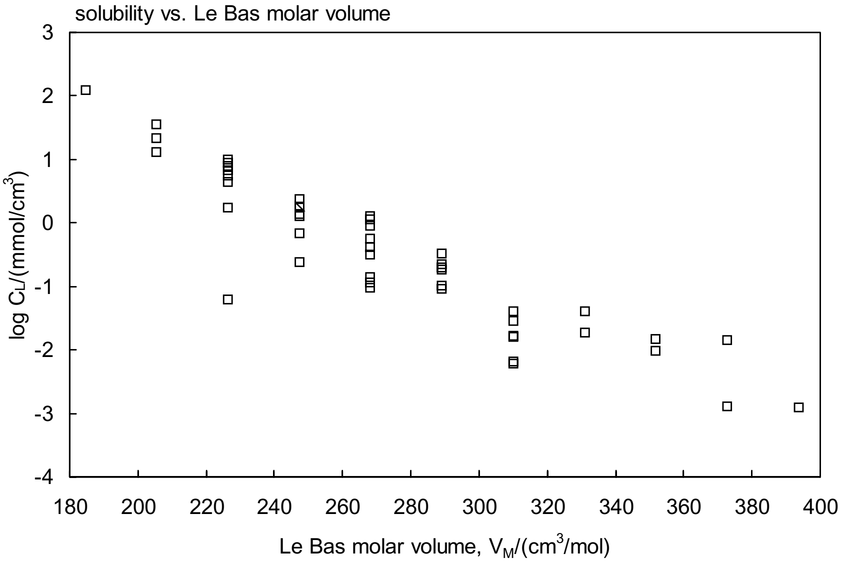


FIGURE 7.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated biphenyls.

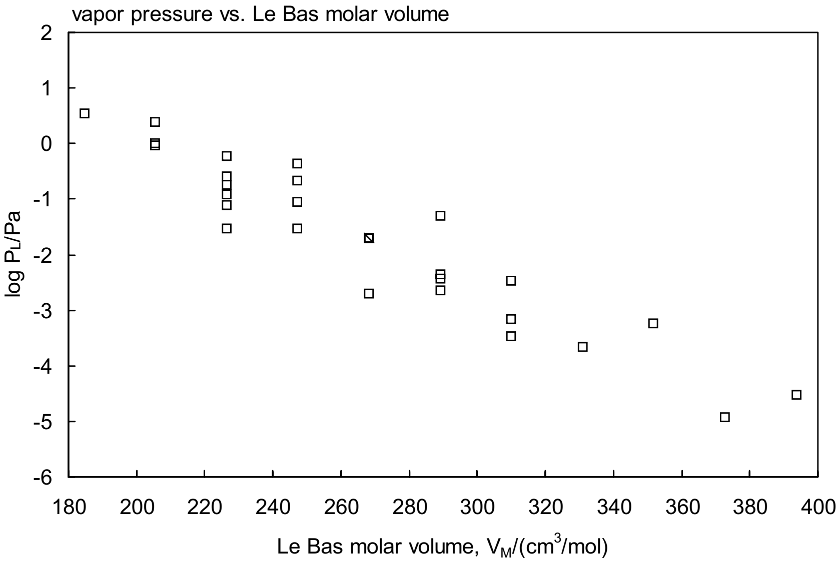


FIGURE 7.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated biphenyls.

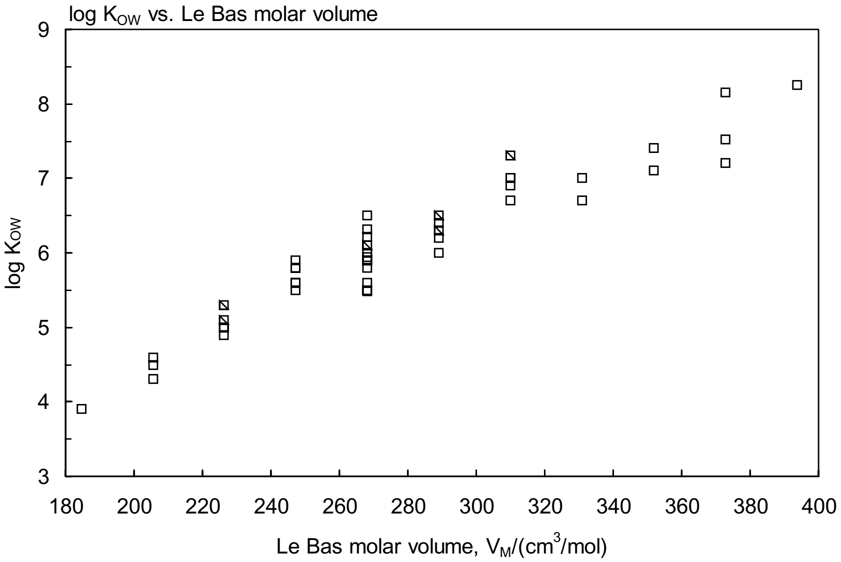


FIGURE 7.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated biphenyls.

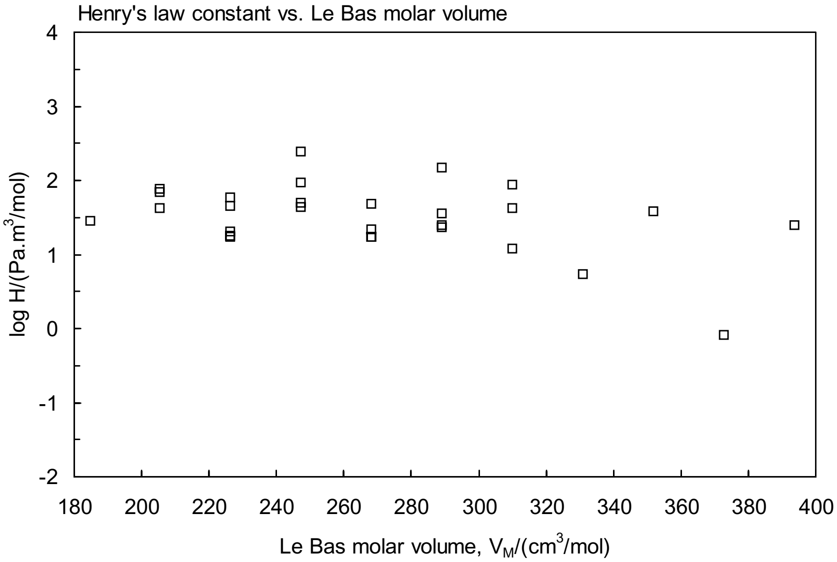


FIGURE 7.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated biphenyls.

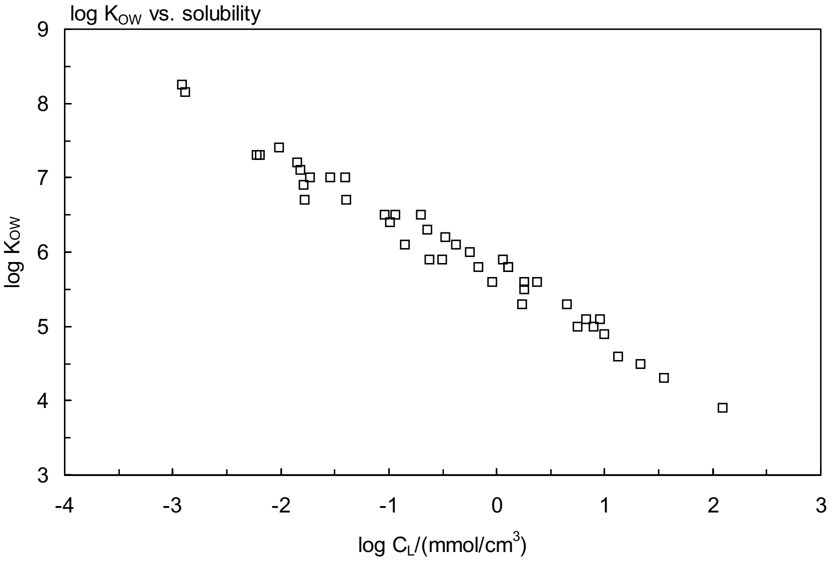


FIGURE 7.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated biphenyls.

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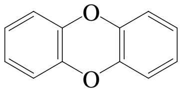
8 Chlorinated Dibenzo-*p*-dioxins

CONTENTS

8.1 LIST OF CHEMICALS AND DATA COMPILATIONS

8.1.1 DIBENZO-*P*-DIOXIN AND CHLORINATED DIBENZO-*P*-DIOXINS

8.1.1.1 Dibenzo-*p*-dioxin



Common Name: Dibenzo-*p*-dioxin
Synonym: dibenzo-1,4-dioxin
Chemical Name: dibenzo-*p*-dioxin
CAS Registry No: 262–12–4
Molecular Formula: $C_6H_4O_2C_6H_4$
Molecular Weight: 184.191
Melting Point (°C):
120.5 (Lide 2003)
Boiling Point (°C):
266.0 (Rordorf 1986)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
143.82, 142.06 (calculated-liquid density, crystalline volume, Govers et al. 1990)
146.96 (liquid molar volume, Govers et al. 1995)
177.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
68.4 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
92.250 (Rordorf 1987)
93.6 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.2, 22.6 (obs., predicted, Rordorf 1986)
22.6 (Ruelle & Kesselring 1997)
23.2, 22.6 (exptl., calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
57 (Rordorf 1986,1987,1989)
58.63, 57.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.116 (mp at 120.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.842*, 0.90 (generator column-HPLC/UV, generator column-GC/ECD; Shiu et al. 1988)
0.90* (generator column-GC/ECD, measured range 4–25°C, Doucette & Andren 1988a)
0.90* (generator column-GC, measured range 4–40°C, Doucette & Andren 1988a)
$S/(mol/L) = 8.85 \times 10^{-7} \exp(0.067 \cdot t/°C)$ (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a)
$\log x = -2541/(T/K) - 1.476$; temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
$\ln x = 4.1680 - 6087.88/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
7.16 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.055* (gas saturation-GC, Rordorf 1985ab, 1986, 1987, 1989)
0.050 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
0.512; 0.251 (supercooled liquid P_L, quoted exptl., calculated-SOFA Solubility-parameter-based-model, Govers & Krop 1998)
$\log (P/Pa) = 14.91018 - 4820.43/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.389; 0.251(GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
0.107* (30°C, Knudsen effusion method, measured range 30–60°C Li et al. 2002)
ln (P/Pa) = (34.944 ± 0.444) – (11259 ± 141)/(T/K); temp range 303–333 K (Knudsen effusion technique, Li et al. 2002, 2004)
ln (P/Pa) = 34.319 – 11095/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):

12.40	(calculated-P/C, Shiu et al. 1987; 1988)
10.96	(calculated-SOFA model, Govers & Krop 1998)
15.85; 10.96	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

4.31, 4.48, 4.38; 4.38, 4.46, 4.52	(HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
4.26, 4.65	(Doucette 1985)
4.17, 4.46	(HPLC-RT correlation, Sarna et al. 1984)
4.26, 4.01; 4.34, 4.17	(HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
4.20	(HPLC-RT correlation, Burkhard & Kuehl 1986)
4.37	(generator column-GC, Doucette & Andren 1987)
4.18	(HPLC-RT correlation, Doucette & Andren 1988b)
4.38	(recommended, Hansch et al. 1995)
4.15	(GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

Bioconcentration Factor, log BCF:

4.49; 4.68 (lipid based BCF, guppy, quoted exptl., calculated-SOFA Solubility-parameter-base-model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

4.34	(sediment/water, calculated-SOFA Solubility-parameter-base-model, Govers & Krop 1998)
4.01	(derived from soot-water distribution coeff., Bärring et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated *data at other temperatures see reference:

$k_{OH} = 4.2 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} corresponding to an atmospheric lifetime τ ~7 h at room temp. (Atkinson 1987a)

$k_{OH}(calc) = 4.0 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987b)

$k_{OH} = 37 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, calculated tropospheric lifetime τ = 0.4 d based on the gas-phase reactions with OH radical and a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} (Atkinson 1991)

$k_{OH} = 1.48 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} and the calculated tropospheric lifetime τ = 1.0 d, $k_{NO3} = 3.9 \times 10^{-27}$ cm^3 $molecule^{-1}$ s^{-1} with calculated lifetime τ = 4.9 d, and $k_{O3} < 5 \times 10^{-20}$ cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime τ >330 d at 297 ± 2 K (Kwok et al. 1994)

$k_{OH}(exptl) = 14.8 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, $k_{OH}(calc) = 9.8 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, corresponding to a tropospheric lifetime of 1.0 d (Kwok et al. 1995)

$k_{OH}* = 12 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 345–385 K; and k_{OH} (calc) = 9.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated atmospheric lifetime τ = 24 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: room temp. gas-phase reaction rate constant k = 4.2×10^{-11} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical corresponding to an atmospheric lifetime of about 7 h (Atkinson 1987a)

tropospheric lifetime τ = 0.4 d calculated for dibenzo-*p*-dioxin based on the gas-phase reaction with OH radical (Atkinson 1991);

tropospheric lifetimes: τ(calc) = 1.0 d, 4.9 d and >330 d for reactions with OH radical, NO_3 radical and O_3, respectively at room temp. (Kwok et al. 1994);

tropospheric lifetime τ(calc) = 1.0 d with respect to reaction with the OH radical (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 8.1.1.1.1

Reported aqueous solubilities and vapor pressures of dibenzo-*p*-dioxin at various temperatures and the reported temperature dependence equations

Aqueous solubility				Vapor pressure			
Shiu et al. 1988		Doucette & Andren 1988		Rordorf 1987, 1989		Li et al. 2002	
generator column-HPLC/UV		generator column-GC/ECD		gas saturation		Knudsen effusion	
t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$	t/°C	P/Pa
5	0.205	4.1	0.212	25	0.055	30	0.107
15	0.460	25	0.90	50	0.98	35	0.215
25	0.842	40	2.392	75	12.0	40	0.358
35	1.762			100	97	45	0.628
45	3.262	$\Delta H_{sol}/(kJ\ mol^{-1})$ = 48.6		125	630	50	1.14
			at 25 °C			55	1.90
$\Delta H_{sol}/(kJ\ mol^{-1})$ = 50.68				$\Delta H_V/(kJ\ mol^{-1})$ = 68.4		60	3.08
	for 5–45 °C	S/(mol/L) = a·exp[b(t/°C)]		$\Delta H_{subl}/(kJ\ mol^{-1})$ = 92.25			
		a	8.85×10^{-7}	$\Delta H_{fus}/(kJ\ mol^{-1})$ = 22.6		ln (P/Pa) = A – B/(T/K)	
		b	0.067	$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1})$ = 57		A	34.994
		OR:				B	11259
		ln *x* = A – B/(T/K)					
		A	–1.476				
		B	2541				

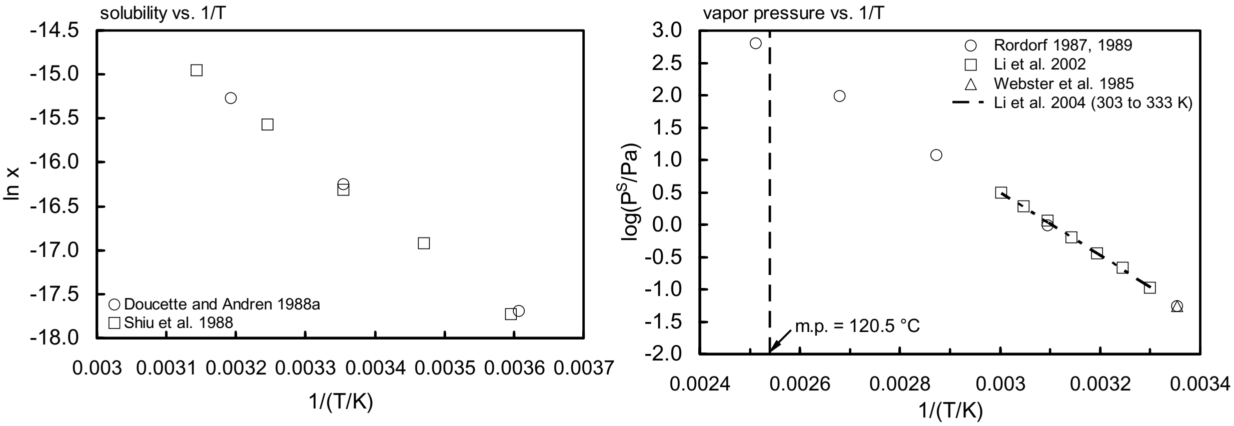
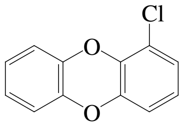


FIGURE 8.1.1.1.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for dibenzo-*p*-dioxin.

8.1.1.2 1-Chlorodibenzo-*p*-dioxin



Common Name: 1-Chlorodibenzo-*p*-dioxin
Synonym: 1-CDD, 1-MCDD
Chemical Name: 1-chlorodibenzo-*p*-dioxin
CAS Registry No: 39227–53–7
Molecular Formula: $C_6H_4O_2C_6H_3Cl$
Molecular Weight: 218.636
Melting Point (°C):
 104.5–105.5 (Pohland & Yang 1972; quoted, Rordorf 1986,1987,1989)
Boiling Point (°C):
 296.0 (Rordorf 1986)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
 157.41, 158.07 (calculated-liquid density, crystalline volume, Govers et al. 1990)
 156.19 (liquid molar volume, Govers et al. 1995)
 197.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 76.2 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
 98.55 (Rordorf 1987)
 100.5 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 23.2, 21.4 (obs., predicted, Rordorf 1986)
 23.2, 22.1 (exptl., calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 56.0 (Rordorf 1986,1987,1989)
 61.34, 58.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.164 (mp at 105.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 0.417* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)
 $\ln x = -0.68385 - 4912.15/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
 1.51 (supercooled liquid S_L, GC-RI correlation; Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 0.012* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989; quoted, Shiu et al. 1988)
 $\log (P/Pa) = 15.35327 - 5150.4/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 0.0275 (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)
 $\ln (P/Pa) = 35.353 - 11859/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
 $\ln (P/Pa) = (36.087 \pm 0.293) - (12085 \pm 96)/(T/K)$; temp range 308–343 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):
 8.38 (calculated-P/C, Shiu et al. 1988)
 6.31; 4.57 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 7.76; 5.75 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

4.97, 5.20, 5.25; 5.05, 5.18, 5.23 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
4.91, 5.18 (HPLC-RT correlation, Sarna et al. 1984)
4.81, 4.52; 4.91, 5.74 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
4.75 (HPLC-RT correlation, Burkhard & Kuehl 1986)
5.05 (recommended, Hansch et al. 1995)
4.99 (GC-RI correlation; Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.86*; 8.34 (generator column-GC; calculated, Harner et al. 2000)
log $K_{OA} = -2.88 + 3200/(T/K)$; temp range 10–40°C (Harner et al. 2000)

Bioconcentration Factor, log BCF:

5.17; 5.08 (lipid wt base, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

5.46 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated *data at other temperatures see reference:
k_{OH}(calc) = 32×10^{-12} cm^3 molecule^{-1} s^{-1}, calculated tropospheric lifetime $\tau = 0.5$ d based on the gas-phase reactions with OH radical and a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 (Atkinson 1991)
k_{OH}(exptl) = 4.7×10^{-12} cm^3·molecule^{-1} s^{-1}, k_{OH}(calc) = 8.3×10^{-12} cm^3 molecule^{-1} s^{-1}, corresponding to a tropospheric lifetime of 1.0 d (relative rate method, Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5$ d calculated for a mono-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);
calculated tropospheric lifetime for mono-chlorinated dioxin was 3.0 d for the gas-phase reaction with OH radical (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

TABLE 8.1.1.2.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1-chlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OA}
5	0.205	25	0.012	10	8.466
15	0.460	50	0.26	20	8.018
25	0.842	75	3.60	30	7.628
35	1.762	100	36.0	40	7.396
45	3.262	125	260	25	7.86
ΔH_{sol}/(kJ mol^{-1}) = 40.85		ΔH_V/(kJ mol^{-1}) = 76.2		log K_{OA} = a + b/(T/K)	
for 5–45°C		ΔH_{subl}/(kJ mol^{-1}) = 98.55		a	–2.88
		ΔH_{fus}/(kJ mol^{-1}) = 21.4		b	3200
		ΔS_{fus}/(J mol^{-1} K^{-1}) = 56.0			
				enthalpy of phase change	
				ΔH_{OA}/(kJ mol^{-1}) = 61.30	

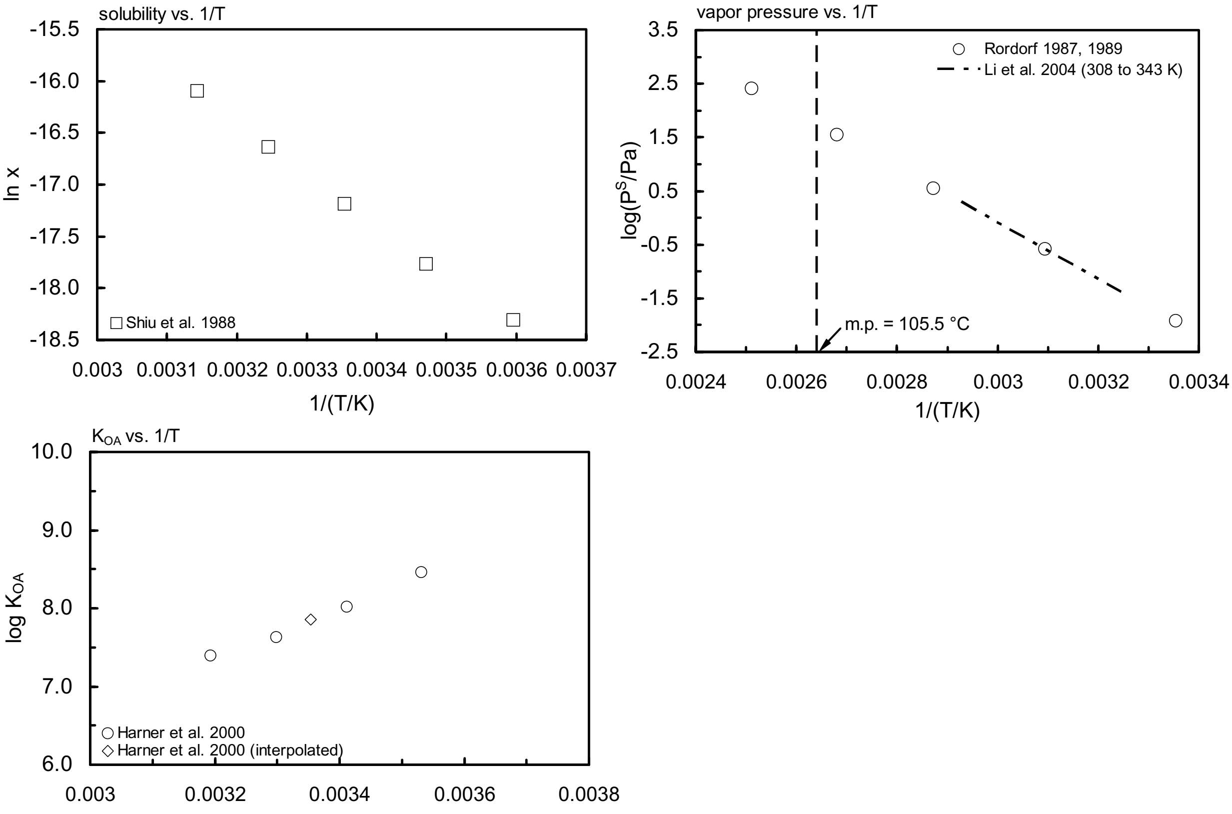
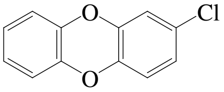


FIGURE 8.1.1.2.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1-chlorodibenzo-*p*-dioxin.

8.1.1.3 2-Chlorodibenzo-*p*-dioxin



Common Name: 2-Chlorodibenzo-*p*-dioxin
Synonym: 2-CDD, 2-MCDD
Chemical Name: 2-chlorodibenzo-*p*-dioxin
CAS Registry No: 39227–54–8
Molecular Formula: $C_6H_4O_2C_6H_3Cl$
Molecular Weight: 218.636
Melting Point (°C):
88–89 (Pohland & Yang 1972)
Boiling Point (°C):
298.0 (Rordorf 1986)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
154.85, 155.15 (calculated-liquid density, crystalline volume, Govers et al. 1990)
153.09 (liquid molar volume, Govers et al. 1995)
197.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
78.2 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
97.16 (Rordorf 1987)
98.1 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.1, 18.5 (obs., predicted, Rordorf 1986)
18.5 (Ruelle & Kesselring 1997)
23.1, 21.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
51 (Rordorf 1987, 1989)
63.78, 57.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.236 (mp at 89°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.278*, 0.319 (generator column-HPLC/UV, generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1988)
0.319* (generator column-GC/ECD, measured range 3.9–39°C, Doucette & Andren 1988a)
$S/(mol/L) = 4.88 \times 10^{-7} \exp(0.048 \cdot t/°C)$ (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
$\log x = -1777/(T/K) - 1.566$, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
$\ln x = 4.093418 - 6448/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
1.44 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.017* (gas saturation-GC, Rordorf 1985a,b,1986,1987,1989)
0.016 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
$\log (P/Pa) = 15.2463 - 5071.88/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.0262 (GC-RI correlation, Wang & Wong 2002)

ln (P/Pa) = 35.106 – 11679/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
ln (P/Pa) = (35.549 ± 0.415) – (11794 ± 134)/(T/K), temp range 308–343 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):
14.82 (calculated-P/C, Shiu et al. 1988)
12.60; 4.57 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
7.586; 4.57 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
5.36, 5.66, 5.71; 5.45, 5.64, 5.69 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
5.45, 5.64 (HPLC-RT correlation, Sarna et al. 1984)
5.33, 5.00; 5.45, 5.29 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
5.08 (HPLC-RT correlation, Burkhard & Kuehl 1986)
4.94 (generator column-GC/ECD, Doucette & Andren 1987)
4.98 (HPLC-RT correlation, Doucette & Andren 1988b)
5.45 (recommended, Hansch et al. 1995)
5.01 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
5.09 (guppy, Loonen et al. 1994)
5.09; 5.12 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:
3.92 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
5.35 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$
Volatilization:
Photolysis: photodegradation $t_{½}$ = 10 min with simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988)
photodegradation k = 1.81 h^{-1} with $t_{½}$ = 0.38 h when loaded on TiO_2 film under UV (λ > 300 nm) or solar light irradiation in the air (Choi et al. 2000).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = 32 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, calculated tropospheric lifetime τ = 0.5 d for a mono-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 (Atkinson 1991)
k_{OH}(exptl) = 4.7×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 9.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 3.0 d at room temp. (relative rate method, Kwok et al. 1995)
k_{OH}(calc) = 4.1×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (Brubaker & Hites 1998)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: tropospheric lifetime τ = 0.5 d calculated for a mono-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);
calculated tropospheric lifetime for mono-chlorinated dioxin was 3.0 d for the gas-phase reaction with OH radical (Kwok et al. 1995).
first-order photodegradation k = 1.81 h^{-1} with $t_{½}$ = 0.38 h when loaded on TiO_2 film under UV (λ > 300 nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: $t_{½}$ = 10 min irradiated under simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988).
Groundwater:
Sediment:
Soil:
Biota:

TABLE 8.1.1.3.1
Reported aqueous solubilities and vapor pressures of 2-chlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure	
Shiu et al. 1988		**Doucette & Andren 1988**		**Rordorf 1987, 1989**	
generator column-HPLC/UV		**generator column-GC/ECD**		**gas saturation-GC**	
t/°C	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**t/°C**	**P/Pa**
5	0.0603	3.9	0.133	25	0.017
15	0.137	25	0.319	50	0.36
25	0.278	39	0.7495	75	4.80
35	0.653			100	45.0
45	1.109			125	320
		ΔH_{sol}/(kJ mol^{-1}) = 34.0			
		4–32 °C		ΔH_V/(kJ mol^{-1}) = 78.1	
ΔH_{sol}/(kJ mol^{-1}) = 53.35				ΔH_{sub}/(kJ mol^{-1}) = 97.16	
5–45 °C				ΔH_{fus}/(kJ mol^{-1}) = 18.5	
				ΔS_{fus}/(J mol^{-1} K^{-1}) = 51	

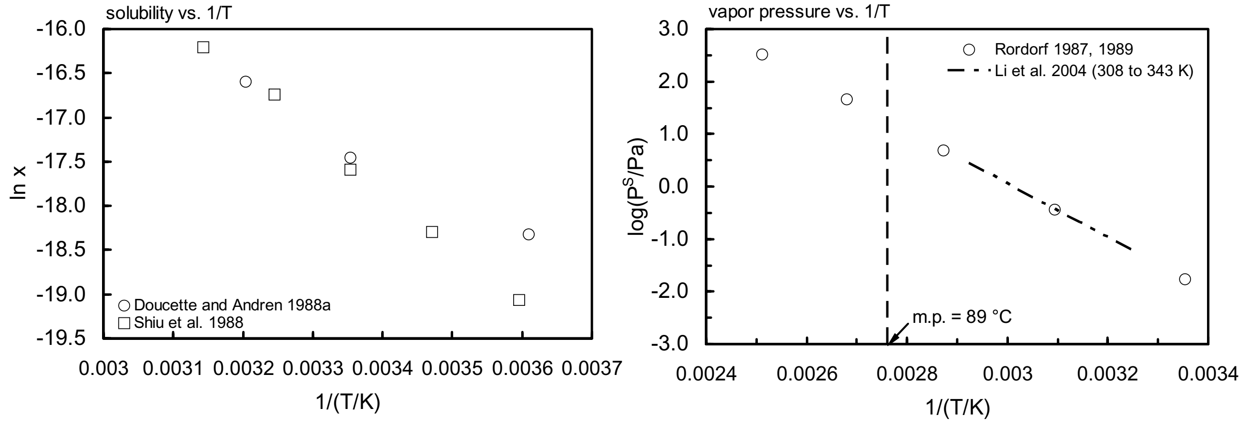
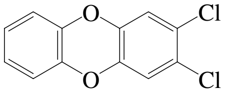


FIGURE 8.1.1.3.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2-chlorodibenzo-*p*-dioxin.

8.1.1.4 2,3-Dichlorodibenzo-*p*-dioxin



Common Name: 2,3-Dichlorodibenzo-*p*-dioxin
Synonym: 2,3-DCDD
Chemical Name: 2,3-dichlorodibenzo-*p*-dioxin
CAS Registry No: 29446–15–9
Molecular Formula: $C_6H_4O_2C_6H_2Cl_2$
Molecular Weight: 253.081
Melting Point (°C):
  163–164 (Pohland & Yang 1972)
Boiling Point (°C):
  358 (calculated, Rordorf 1986,1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  164.07 (calculated-liquid density, Govers et al. 1990)
  162.67 (liquid molar volume, Govers et al. 1995)
  218.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  77.8 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
  106.23 (Rordorf 1987)
  106.2 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  26.7 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  61 (Rordorf 1986,1987,1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0433 (mp at 164°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.0149* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)
  $\ln x = 0.07859 - 6173.64/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
  0.297 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.00039* (gas saturation-GC, Rordorf 1985a,b, 1986,1989)
  0.0004 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
  0.0020 (GC-RI correlation, Wang & Wong 2002)
  $\log (P_L/\text{mmHg}) = 48.98 - 6446/(T/K) - 12.569 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
  $\ln (P/\text{Pa}) = 35.096 - 12804/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
  $\ln (P/\text{Pa}) = (35.081 \pm 0.374) - (12771 \pm 134)/(T/K)$; temp range 338–378 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):
  6.61 (calculated-P/C, Shiu et al. 1988)
  6.61; 2.51 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
  3.80; 2.51 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

4.70 (calculated, Kaiser 1983)
6.23, 5.60 (calculated-QSAR, quoted, Fiedler & Schramm 1990)
5.77 (calculated-SOFA model, Govers & Krop 1998)
5.738 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
5.80; 5.77 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

8.50 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.41 (lipid wt based, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

4.73 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
6.27 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 22×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)
k_{OH} = (22 - 28) $\times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, calculated tropospheric lifetime τ = 0.5–0.7 d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} (Atkinson 1991)
k_{OH}(calc) = (5.9 - 7.3) $\times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with a calculated tropospheric lifetime τ = 2.0–2.4 d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)
k_{OH}(calc) = 4.1×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Brubaker & Hites 1998)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.092 d^{-1} (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.5–0.7 d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);
calculated tropospheric lifetime τ = 2.0–2.4 d for the reaction with OH radical (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: mean biological $t_{1/2}$ ~2 d in rainbow trout (Niimi 1986);
biological $t_{1/2}$ = 7 d in rainbow trout (Niimi & Oliver 1986);
biological $t_{1/2}$ = 2–7 d in trout (Niimi 1987).

TABLE 8.1.1.4.1
Reported aqueous solubilities and vapor pressures of 2,3-dichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure	
Shiu et al. 1988		Rordorf 1987, 1989	
generator column-HPLC/UV		gas saturation-GC	
t/°C	$S/g \cdot m^{-3}$	t/°C	P/Pa
5	0.00368	25	0.00039
15	0.00716	50	0.0011
25	0.0149	75	0.18
35	0.0304	100	2.20
45	0.0586	125	19.0
		$\Delta H_V/(kJ\ mol^{-1}) = 77.8$	
$\Delta H_{sol}/(kJ\ mol^{-1}) = 51.3$		$\Delta H_{subl}/(kJ\ mol^{-1}) = 106.23$	
5–45 °C		$\Delta H_{fus}/(kJ\ mol^{-1}) = 26.7$	
		$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1}) = 61$	

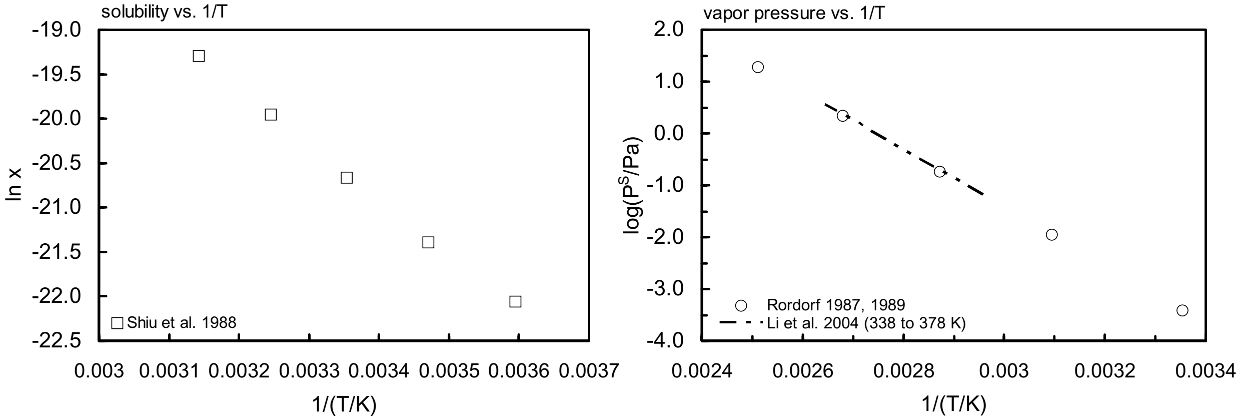
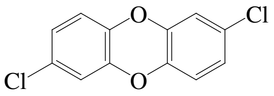


FIGURE 8.1.1.4.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,3-dichlorodibenzo-*p*-dioxin.

8.1.1.5 2,7-Dichlorodibenzo-*p*-dioxin



Common Name: 2,7-Dichlorodibenzo-*p*-dioxin
Synonym: 2,7-DCDD
Chemical Name: 2,7-dichlorodibenzo-*p*-dioxin
CAS Registry No: 33857–26–0
Molecular Formula: $ClC_6H_3O_2C_6H_3Cl$
Molecular Weight: 253.081
Melting Point (°C):
210 (Lide 2003)
Boiling Point (°C):
374.5 (calculated, Rordorf 1987, 1989)
Density (g/cm^3):
1.647 (calculated, Boer et al. 1972)
Molar Volume (cm^3/mol):
165.88, 162.89 (calculated-liquid density, crystalline volume, Govers et al. 1990)
162.87 (liquid molar volume, Govers et al. 1995)
218.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
76.4 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
105.51 (Rordorf 1987)
113.8 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
26.8 (Rordorf 1986, 1987; Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
55 (Rordorf 1986,1987,1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0188 (mp at 201°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00375* (generator column-HPLC/UV, Shiu et al. 1988)
0.00224 (generator column-GC/MS, Santl et al. 1994)
$\ln x = -3.48833 - 5543.9/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.311 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00012* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989; quoted, Shiu et al. 1988)
0.00013 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
$\log (P/Pa) = 14.60827 - 5523.34/(T/K)$ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.00219 (GC-RI correlation, Wang & Wong 2002)
$\log (P_L/mmHg) = 49.61 - 6624/(T/K) - 12.569\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
$\ln (P/Pa) = 33.637 - 12718/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
$\ln (P/Pa) = (36.293 \pm 0.648) - (13686 \pm 245)/(T/K)$; temp range 358–393 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):

8.11 (calculated-P/C, Shiu et al. 1988)
6.98 (gas stripping-GC/MS, Santl et al. 1994)
8.13; 2.82 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
3.89; 2.82 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

6.28, 6.64, 6.72; 6.38, 6.62, 6.71 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
6.62, 6.39 (HPLC-RT correlation, Sarna et al. 1984)
6.27, 5.86; 6.39, 6.17 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
5.75 (HPLC-RT correlation, Burkhard & Kuehl 1986)
6.38 (recommended, Sangster 1993)
6.38 (recommended, Hansch et al. 1995)
5.77 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.36*; 8.67 (generator column-GC; calculated, Harner et al. 2000)
log K_{OA} = –3.74 + 3610/(T/K); temp range 10–40°C (Harner et al. 2000)
8.48 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

1.7, 2.9 (guppy, in whole fish, in lipid, Gobas et al. 1987)
2.56, 3.68 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
5.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

6.15 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photodegradation $t_{½}$ = 46 min in an aqueous solution assisted by TiO_2 at 2.0 g/L under simulated sunlight (Barbeni et al. 1986)

photodegradation $t_{½}$ = 1 h with irradiation under simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988)

photolysis k = 8.9×10^{-2} min^{-1} with $t_{½}$ = 7.8 min in pure water, and rate constant k = 0.16 min^{-1} with $t_{½}$ = 4.3 min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (26–28) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (22–28) × 10^{-12} cm^3 molecule^{-1} s^{-1}, calculated tropospheric lifetime τ = 0.5–0.7 d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 (Atkinson 1991)

k_{OH}(calc) = (5.9–7.3) × 10^{-12} cm^3 molecule^{-1} s^{-1} with a calculated tropospheric lifetime τ = 2.0–2.4 d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

k_{OH}(calc) = 4.1×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Brubaker & Hites 1998)

k_{OH}* = 23×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, measured temp range 355–395 K, and k_{OH}(calc) = 4.1×10^{-12} cm^3 molecule^{-1} s^{-1},with a calculation lifetime τ = 65 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Biodegradation:

Biotransformation: metabolic elimination k_m = 0.23 d^{-1} (goldfish, 20°C, 96-h exposure, Sijm & Opperhuizen 1988)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.462 d^{-1} (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)
k_1 = 390 mL g^{-1} d^{-1}; k_2 = 0.23 d^{-1} (goldfish, 20°C, 96-h exposure, Sijm & Opperhuizen 1988)
k_1 = 543 d^{-1}; k_2 = 1.5 d^{-1} (guppy, Gobas & Schrap 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.5–0.7 d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);
tropospheric calculated lifetime τ = 2.0–2.4 d for the reaction with OH radical (Kwok et al. 1995);
calculated lifetime τ = 65 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: photodegradation $t_{1/2}$ = 1 h with irradiation under simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988);
photolysis rate constant k = 8.9×10^{-2} min^{-1} with $t_{1/2}$ = 7.8 min in pure water, and k = 1.6×10^{-1} min^{-1} with $t_{1/2}$ = 4.3 min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000).

Groundwater:

Sediment:

Soil:

Biota: mean biological $t_{1/2}$ ~ 2 d in rainbow trout (Niimi 1986);
biological $t_{1/2}$ = 2 d in rainbow trout (Niimi & Oliver 1986);
biological $t_{1/2}$ = 2–7 d in trout (Niimi 1987).

TABLE 8.1.1.5.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,7-dichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OA}
5	0.00109	25	0.0001	10	9.020
15	0.00201	50	0.0033	20	8.564
25	0.00375	75	0.056	30	8.106
35	0.00727	100	0.64	40	7.818
45	0.0134	125	5.4	25	7.36
		ΔH_V/(kJ mol^{-1}) = 76.4		log K_{OA} = a + b/(T/K)	
ΔH_{sol}/(kJ mol^{-1}) = 50.68		ΔH_{subl}/(kJ mol^{-1}) = 105.51		a	−3.74
25 °C		ΔH_{fus}/(kJ mol^{-1}) = 26.8		b	3610
		ΔS_{fus}/(J mol^{-1} K^{-1}) = 55			
				enthalpy of phase change	
				ΔH_{OA}/(kJ mol^{-1}) = 69.0	

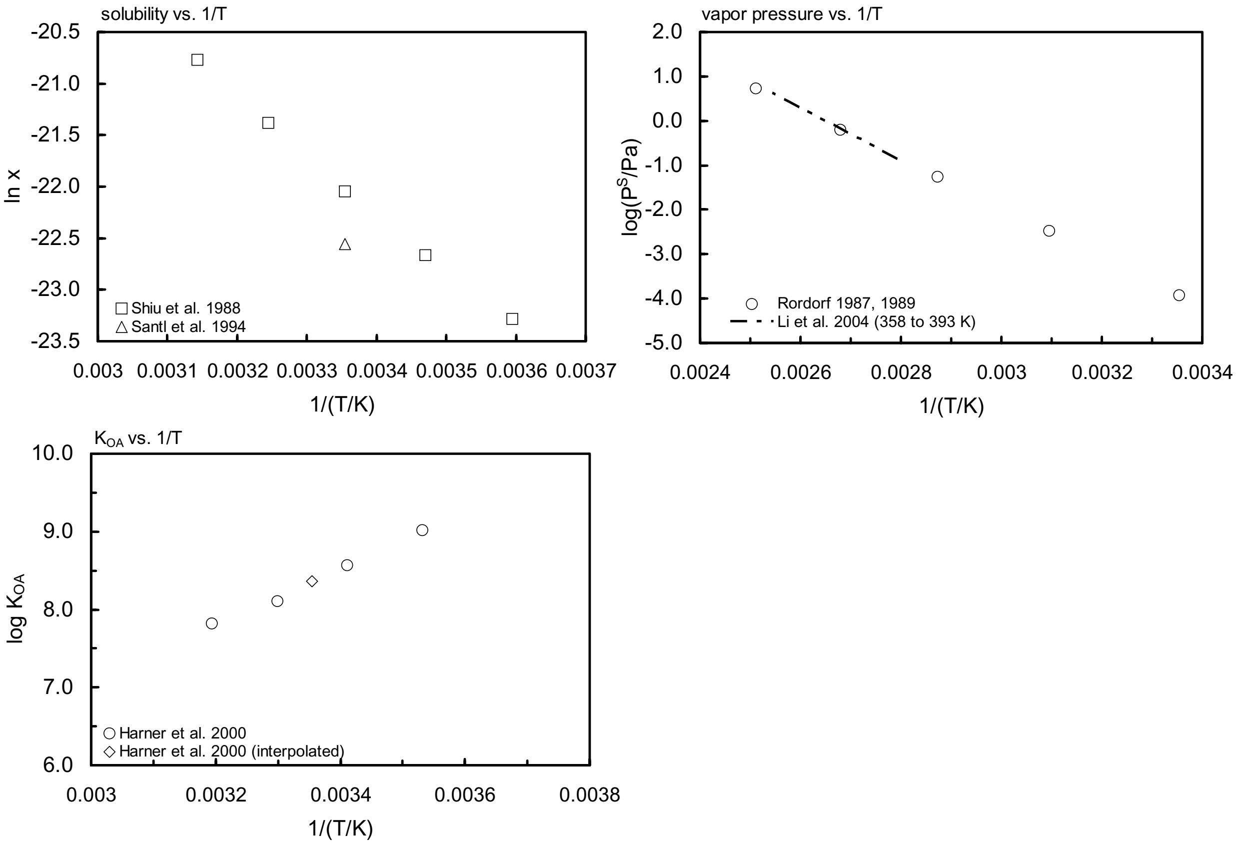
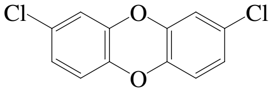


FIGURE 8.1.1.5.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,7-dichlorodibenzo-*p*-dioxin.

8.1.1.6 2,8-Dichlorodibenzo-*p*-dioxin



Common Name: 2,8-Dichlorodibenzo-*p*-dioxin
Synonym: 2,8-TCDD
Chemical Name: 2,8-dichlorodibenzo-*p*-dioxin
CAS Registry No: 38964–22–6
Molecular Formula: $ClC_6H_3O_2C_6H_3Cl$
Molecular Weight: 253.081
Melting Point (°C):
150.5–151 (Pohland & Yang 1972; Rordorf 1986,1987,1989)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
165.88, 167.2 (calculated-liquid density, crystalline volume, Govers et al. 1990)
160.63 (liquid molar volume, Govers et al. 1995)
218.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
84.1 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
109.01 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.2 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
55 (Rordorf 1986,1987,1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.058 (mp at 151°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0167* (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1988)
$\ln x = -2.54177 - 5379/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.311 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00014* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989)
0.00013 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
$\log (P/Pa) = 15.25386 - 5699.96/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.00219 (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)
0.00150 (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
0.0260 (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
$\log (P_L/mmHg) = 49.89 - 6705/(T/K) - 12.569 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C):
2.13 (calculated-P/C, Shiu et al. 1988)
2.14; 2.29 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
3.89; 2.29 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

4.70 (calculated, Kaiser 1983)
5.60 (selected, Shiu et al. 1988)
5.68 (calculated-SOFA model, Govers & Krop 1998)
5.638 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
5.77; 5.68 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
5.34, 5.50, 5.75, 5.58 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.36*; 8.65 (generator column-GC; measured range 10–40°C; calculated, Harner et al. 2000)
$\log K_{OA} = -3.74 + 3610/(T/K)$; temp range 10–40°C, (Harner et al. 2000)
8.48 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

2.77, 2.82 (goldfish: treated with metabolic inhibitor PBO, untreated, Sijm & Opperhuizen 1988)
5.42 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

6.14 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(26–28) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)
k_{OH} = $(22–28) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, calculated tropospheric lifetime τ = 0.5–0.7 d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 (Atkinson 1991)
k_{OH}(calc) = $(5.9–7.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with a calculated tropospheric lifetime τ = 2.0–2.4 d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)
Biodegradation:
Biotransformation: metabolic elimination rate constant from goldfish was estimated to be 0.35 d^{-1} (Sijm & Opperhuizen 1988).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 390 L kg^{-1}·d^{-1}; k_2 = 0.23 d^{-1} (goldfish, Opperhuizen & Sijm 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.5 – 0.7 d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);
calculated tropospheric lifetime τ = 2.0 – 2.4 d for the reaction with OH radical. (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: mean biological $t_{½}$ ~ 2 d in rainbow trout (Niimi 1986);
biological $t_{½}$ = 2–7 d in trout (Niimi 1987).

TABLE 8.1.1.6.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,8-dichlorodibenzo-*p*-dioxon at various temperatures

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
t/°C	$S/g \cdot m^{-3}$			t/°C	log K_{OA}
5	0.00422	25	0.0001	10	9.020
15	0.00859	50	0.0042	20	8.564
25	0.0167	75	0.078	30	8.106
35	0.0275	100	0.97	40	7.818
45	0.0515	125	8.80	25	8.36
		$\Delta H_V/(kJ\ mol^{-1}) = 84.1$		log K_{OA} = a + b/(T/K)	
$\Delta H_{sol}/(kJ\ mol^{-1}) = 50.04$		$\Delta H_{subl}/(kJ\ mol^{-1}) = 109.01$		a	–3.74
5–45 °C		$\Delta H_{fus}/(kJ\ mol^{-1}) = 23.3$		b	3610
		$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1}) = 55$			
				enthalpy of phase change	
				$\Delta H_{OA}/(kJ\ mol^{-1}) = 69.0$	

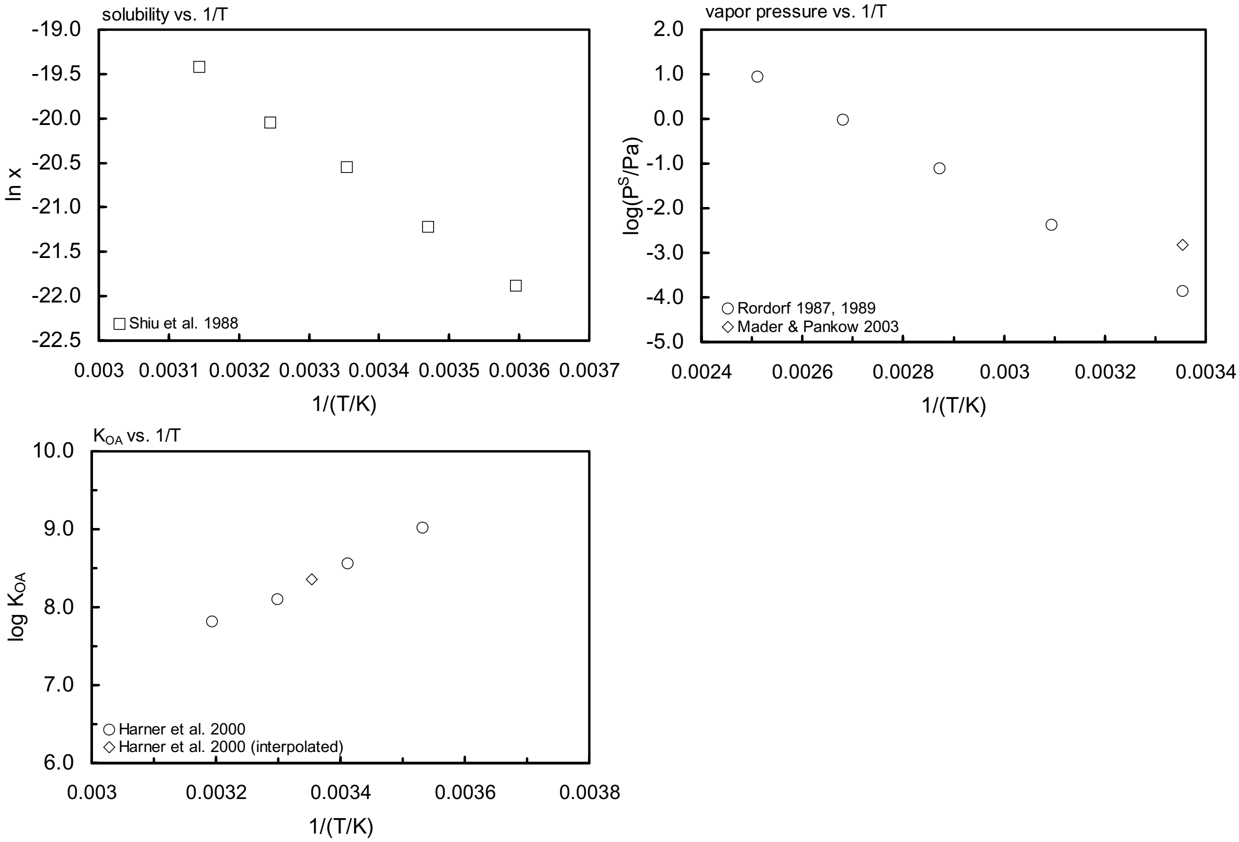
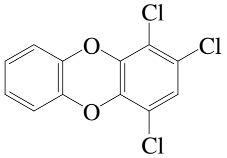


FIGURE 8.1.1.6.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,8-dichlorodibenzo-*p*-dioxin.

8.1.1.7 1,2,4-Trichlorodibenzo-*p*-dioxin



Common Name: 1,2,4-Trichlorodibenzo-*p*-dioxin
Synonym: 1,2,4-TCDD
Chemical Name: 1,2,4-trichlorodibenzo-*p*-dioxin
CAS Registry No: 39227–58–2
Molecular Formula: $C_{12}H_5Cl_3O_2$, $C_6H_4O_2C_6HCl_3$
Molecular Weight: 287.526
Melting Point (°C):
128–129 (Pohland & Yang 1972; quoted, Rordorf 1986, 1987, 1989)
Boiling Point (°C):
375.0 (calculated, Rordorf 1986,1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
179.66 (calculated-liquid density, Govers et al. 1990)
173.60 (liquid molar volume, Govers et al. 1995)
239.7 (calculated-Le Bas method at normal boiling)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
83.9 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
118.79 (Rordorf 1987)
121.0 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
33.9 (Rordorf 1986, 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
67 (Rordorf 1986,1987,1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0954 (mp at 129°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00841* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)
0.00695 (generator column-GC/MS, Santl et al. 1994)
$\ln x = -2.4909 - 5626.95/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.091 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0001* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989)
0.0001 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
$\log (P/Pa) = 16.9148 - 6235.45/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.000324 (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)
5.07×10^{-4} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
5.43×10^{-3} (supercooled liquid P_L, calculated from measured P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
$\log (P_L/mmHg) = 47.18 - 6479/(T/K) - 12.028 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/Pa) = 38.948 - 14358/(T/K)$; temp range 298 – 398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
$\ln(P/Pa) = (39.303 \pm 0.605) - (14550 \pm 221)/(T/K)$; temp range 348–383 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):

3.84	(calculated-P/C, Shiu et al. 1988)
3.64	(gas stripping-GC/MS, Santl et al. 1994)
3.72; 1.82	(quoted exptl., calculated-SOFA model, Govers & Krop 1998)
2.29; 1.82	(GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

7.40, 7.77, 7.69; 7.47, 7.76, 7.68 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
7.45, 7.76 (HPLC-RT correlation, Sarna et al. 1984)
7.36, 6.86; 7.45, 7.11 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)

6.45	(HPLC-RT correlation, Burkhard & Kuehl 1986)
7.47	(recommended, Hansch et al. 1995)
6.34	(GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

8.97	(GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

1.90, 3.10	(guppy, in whole fish, in lipid, Gobas et al. 1987)
2.82, 3.95	(guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
5.42	(lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

7.01	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
5.87	(derived from soot-water distribution coeff., Bärring et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is 1.27×10^6 L g^{-1} min^{-1} under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = $(21–22) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(17–22) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, calculated tropospheric lifetime $\tau = 0.7–0.9$ d for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 (Atkinson 1991)

k_{OH}(calc) = $(4.5–5.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime $\tau = 2.5–3.3$ d for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.058$ d^{-1} (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

$k_1 = 601$ d^{-1}; $k_2 = 0.91$ d^{-1} (guppy, Gobas & Schrap 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.7–0.9$ d calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radical (Atkinson 1991); the calculated tropospheric lifetime $\tau = 2.5–3.3$ d for the gas phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone k = 1.27×10^6 L g^{-1} min^{-1} under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987).

Sediment:
Soil:
Biota: mean biological $t_{½}$ ~ 10 d in rainbow trout (Niimi 1986);
$t_{½}$ = 12 d in rainbow trout (Niimi & Oliver 1986);
biological $t_{½}$ = 12 d in trout (Niimi 1987)

TABLE 8.1.1.7.1
Reported aqueous solubilities and vapor pressures of 1,2,4-trichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		**Vapor pressure**	
Shiu et al. 1988		**Rordorf 1987, 1989**	
generator column-HPLC/UV		**gas saturation-GC**	
t/°C	**S/g·m^{-3}**	**t/°C**	**P/Pa**
5	0.00219	25	0.0001
15	0.00477	50	0.0042
25	0.00841	75	0.1
35	0.0167	100	1.6
45	0.0282	125	18
		ΔH_V/(kJ mol^{-1}) = 83.9	
ΔH_{sol}/(kJ mol^{-1}) = 46.62		ΔH_{subl}/(kJ mol^{-1}) = 118.79	
5–45 °C		ΔH_{fus}/(kJ mol^{-1}) = 33.9	
		ΔS_{fus}/(J mol^{-1} K^{-1}) = 84	

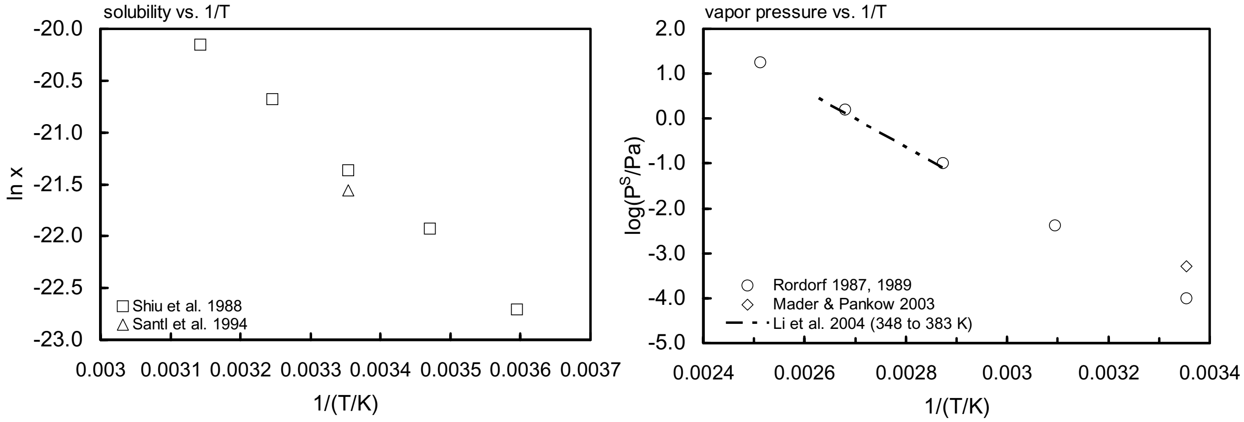
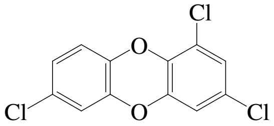


FIGURE 8.1.1.7.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,4-trichlorodibenzo-*p*-dioxin.

8.1.1.8 1,3,7-Trichlorodibenzo-*p*-dioxin



Common Name: 1,3,7-Trichlorodibenzo-*p*-dioxin
Synonym: 1,3,7-TCDD
Chemical Name: 1,3,7-trichlorodibenzo-*p*-dioxin
CAS Registry No: 67026–17–5
Molecular Formula: $C_{12}H_5Cl_3O_2$, $ClC_6H_3O_2C_6H_2Cl_2$
Molecular Weight: 287.526
Melting Point (°C):
148.5 (Rordorf 1986, 1987, 1989)
Boiling Point (°C):
398 (calculated, Rordorf 1986,1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
170.18 (liquid molar volume, Govers et al. 1995)
239.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
86.4 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
116.2 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.4 (Rordorf 1986, 1987)
30.8, 25.7 (reported exptl., calculated, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
67 (Rordorf 1986,1987,1989)
73.04, 61.0 (reported exptl., calculated, Chickos 1999)
Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 0.0614 (mp at 148.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0974 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0997; 0.0974 (supercooled liquid S_L, GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3.60×10^{-5}* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989)
3.63×10^{-4} (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)
$\log (P_L/\text{mmHg}) = 48.01 - 6714/(T/K) - 12.028 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C):
1.48 (calculated-SOFA model, Govers & Krop 1998)
2.34, 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.19 (calculated-SOFA model, Govers & Krop 1998)
6.31; 6.19 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

5.55 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

6.85 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is 1.27×10^6 L g^{-1} min^{-1} under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = $(21–22) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(17–22) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, calculated tropospheric lifetime τ = 0.7–0.9 d for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 (Atkinson 1991)

k_{OH}(calc) = $(4.5–5.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 2.5–3.3 d for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.7–0.9 d calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); the calculated tropospheric lifetime τ = .5–3.3 d for the gas phase reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone k = 1.27×10^6 L·g^{-1}·min^{-1} under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987).

Sediment:

Soil:

Biota:

TABLE 8.1.1.8.1
Reported vapor pressures of 1,3,7-trichlorodibenzo-*p*-dioxin at various temperatures

Rordorf 1987, 1989	
gas saturation-GC/ECD	
t/°C	P/Pa
25	3.6×10^{-5}
50	1.4×10^{-3}
75	3.1×10^{-2}
100	0.45
125	4.70
ΔH_V/(kJ mol^{-1}) = 86.4	
ΔH_{subl}/(kJ mol^{-1}) = 116.2	
ΔH_{fus}/(kJ mol^{-1}) = 28.4	

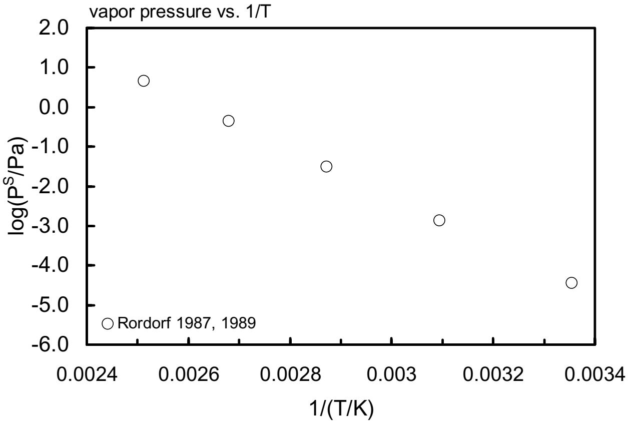
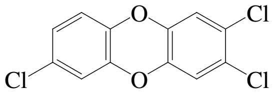


FIGURE 8.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3,7-trichlorodibenzo-*p*-dioxin.

8.1.1.9 2,3,7-Trichlorodibenzo-*p*-dioxin



Common Name: 2,3,7-Trichlorodibenzo-*p*-dioxin
Synonym: 2,3,7-TCDD
Chemical Name: 2,3,7-trichlorodibenzo-*p*-dioxin
CAS Registry No: 33857–28–2
Molecular Formula: $C_{12}H_5Cl_3O_2$, $ClC_6H_3O_2C_6H_2Cl_2$
Molecular Weight: 287.526
Melting Point (°C):
162–163 (Rordorf 1986, 1987, 1989)
Boiling Point (°C):
408.4 (calculated, Rordorf 1986,1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
179.11 (calculated-liquid density, Govers et al. 1990)
239.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
88.2 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
119.759 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
30.9 (Rordorf 1986, 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
71 (Rordorf 1986,1987,1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0548 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0674; 0.0548 (supercooled liquid S_L, GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.000012* (calculated, Rordorf 1985a,b,1986,1987,1989)
2.14×10^{-4} (supercooled liquid P_L, GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
$\log (P_L/\text{mmHg}) = 48.21 - 6829/(T/K) - 12.028\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C):
1.78 (calculated-SOFA model, Govers & Krop 1998)
2.04; 1.78 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.33 (calculated-SOFA model, Govers & Krop 1998)
6.46; 6.33 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
6.47 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
9.14*, 9.28 (generator column-GC/ECD, measured range 0–40°C, calculated, Harner et al. 2000)
$\log K_{OA} = -5.35 + 4320/(T/K)$ (generator column-GC/ECD, measured range 0–40°C, Harner et al. 2000)
9.42 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.52 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

7.05 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolysis rate $k = 2.03 \times 10^{-4}$ s^{-1} at 313 nm using a Hanovia 450-W mercury lamp in hexane solution (Dulin et al. 1986)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is 1.27×10^6 L g^{-1} min^{-1} under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = (21–22) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (17–22) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, calculated tropospheric lifetime τ = 0.7–0.9 d for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 (Atkinson 1991)

k_{OH}(calc) = (4.5–5.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 2.5–3.3 d for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.7 – 0.9 d calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric lifetime τ(calc) = 2.5 – 3.3 d for the gas phase reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone $k = 1.27 \times 10^6$ $L \cdot g^{-1} \cdot min^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987).

Sediment:

Soil:

Biota:

TABLE 8.1.1.9.1
Reported vapor pressures and octanol-air partition coefficients of 2,3,7-trichlorodibenzo-*p*-dioxin at various temperatures

Vapor pressure		log K_{OA}	
Rordorf 1987, 1989		Harner et al. 2000	
vapor pressure correlation		generator column-GC/ECD	
t/°C	P/Pa	t/°C	K_{OA}
25	1.2×10^{-5}	0	10.573
50	5.2×10^{-4}	10	9.816
75	1.3×10^{-2}	20	9.313
100	0.21	30	8.935
125	2.3	40	8.497
		25	9.28
$\Delta H_V/(kJ\ mol^{-1}) = 87.2$			
$\Delta H_{subl}/(kJ\ mol^{-1}) = 119.76$		log K_{OA} = a + b/(T/K)	
$\Delta H_{fus}/(kJ\ mol^{-1}) = 30.9$		a	–5.35
		b	4320
		$\Delta H_{OA}/(kJ\ mol^{-1}) = 82.7$	

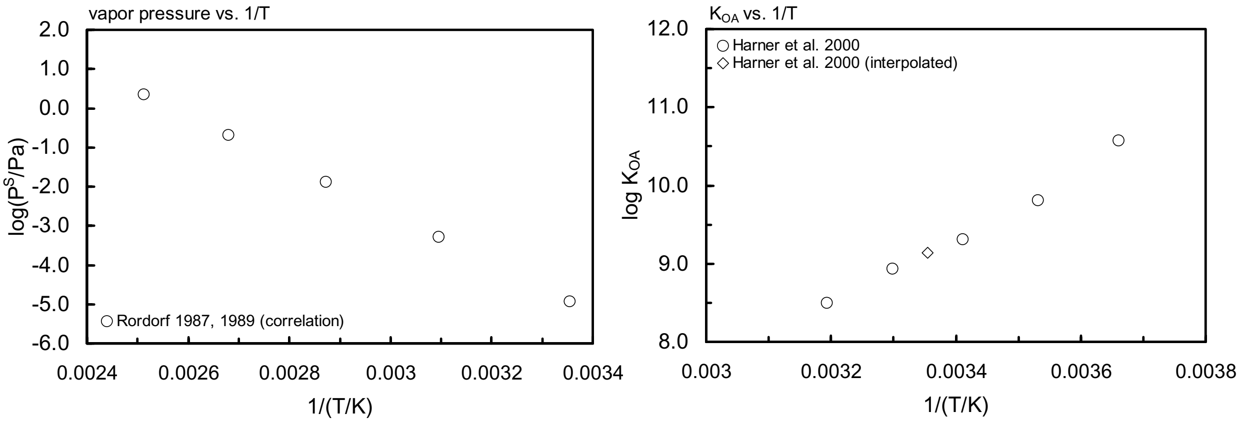
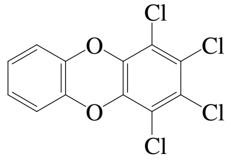


FIGURE 8.1.1.9.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 2,3,7-trichlorodibenzo-*p*-dioxin.

8.1.1.10 1,2,3,4-Tetrachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,4-Tetrachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,4-TCDD
Chemical Name: 1,2,3,4-tetrachlorodibenzo-*p*-dioxin
CAS Registry No: 30746–58–8
Molecular Formula: $C_6H_4O_2C_6Cl_4$
Molecular Weight: 321.971
Melting Point (°C):
189 (Pohland & Yang 1972; Rordorf 1986,1987,1989)
Boiling Point (°C):
419 (calculated, Rordorf 1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
186.71 (calculated-liquid density, Govers et al. 1990)
186.10 (liquid molar volume, Govers et al. 1995)
260.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
85.6 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
118.53 (Rordorf 1987)
111.3 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
31.2 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
68 (Rordorf 1986,1987,1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0246 (mp at 189°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00063*, 0.00047 (generator column-HPLC/UV, generator column-GC/ECD, Shiu et al. 1988)
0.00047* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988a)
$S/(\text{mol/L}) = 2.75 \times 10^{-10} \exp(0.065 \cdot t/°C)$ (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
$\log x = -2447/(T/K) - 2.373$, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
0.000388 (generator column-GC/MS, Santl et al. 1994)
$\ln x = -10.5076 - 3984/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0165 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0000064* (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)
1.00×10^{-5} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
1.04×10^{-4} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)
6.30×10^{-6} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
6.37×10^{-4} (corrected supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1998)
2.48×10^{-6} (solid vapor pressure calculated from reported P_L, Delle Site 1997)
$\log (P/\text{Pa}) = 15.59851 - 6199.79/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
2.75×10^{-5} (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)

2.26×10^{-5} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
9.66×10^{-4} (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
$\log (P_L/\text{mmHg}) = 45.97 - 6777/(T/K) - 11.499 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
$\ln (P/Pa) = 35.917 - 14276/(T/K)$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
$\ln (P/Pa) = (33.217 \pm 0.442) - (13386 \pm 173)/(T/K)$; temp range 378–403 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):
3.77 (calculated-P/C, Shiu et al. 1988)
2.02 (gas stripping-GC/MS, Santl et al. 1994)
3.02; 1.35 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
1.15; 1.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
8.65, 8.90, 8.96; 8.66, 8.91, 8.97 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
8.64, 8.91 (HPLC-RT correlation, Sarna et al. 1984)
8.63, 8.02; 8.64, 8.07 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
7.18, 7.08 (HPLC-RT correlation, Burkhard & Kuehl 1986)
6.20 (generator column-GC/ECD, Doucette & Andren 1987)
6.85 (HPLC-RT correlation, Doucette & Andren 1988b)
6.48 (shake flask/slow stirring method-GC/ECD, mixture from fly-ash extract, Sijm et al. 1989a)
7.18 (recommended, Sangster 1993)
7.18 (recommended, Hansch et al. 1995)
7.04 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
9.410 (calculated-K_{OW}/K_{AW}, Paterson et al. 1991)
9.70*; 9.86 (generator column-GC; calculated, Harner et al. 2000)
$\log K_{OA} = -4.96 + 4370/(T/K)$; temp range 10–40°C (Harner et al. 2000)
9.64 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:
2.20, 3.40 (guppy, in whole fish, in lipid, Gobas et al. 1987)
2.90, 4.02 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
5.52 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:
7.88 (sediment/water., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Photolysis: solution photolysis $t_{1/2}$ =1294 min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2}$ = 560 min on a clean glass surface under the same conditions (Nestrick et al. 1980)
sunlight induced photolysis $t_{1/2}$ = 380 min in isooctane solution and sunlight induced solid phase $t_{1/2}$ = 65 h of TCDD dispersed as solid films (Buser 1988);
photodegradation $t_{1/2}$ = 88 h for 1,2,3,4-TCDD adsorbed to clean silica gels in a rotary photo-reactor by filtered <290 nm of light (Koester & Hites 1992);
first-order photodegradation k = 0.98 h^{-1} with $t_{1/2}$ = 0.71 h when loaded on TiO_2 film under UV (λ > 300 nm) or solar light irradiation in the air (Choi et al. 2000)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k (oxidative degradation rate of water dissolved PCDD by ozone) is 4.73×10^5 L g^{-1} min^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)
k_{OH}(calc) = $(16 - 19) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (7.6 – 19) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5 × 10^6 molecule/cm^3 at room temp. (Atkinson 1991)

k_{OH}(calc) = (2.0 – 5.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 2.8–7.2 d for a tri-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

k_{OH}* = 8.5 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 306 – 366 K (Brubaker & Hites 1997)

k_{OH}(calc) = 8 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K (Brubaker & Hites 1998)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.016 d^{-1} (rainbow trout, Niimi & Oliver 1986)

k_1 = 953 d^{-1}; k_2 = 1.20 d^{-1} (guppy, Gobas & Schrap 1990)

k_1 = 35 L kg^{-1} d^{-1}; k_2 > 0.23 d^{-1} (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 66 L kg^{-1} d^{-1}, 104 L kg^{-1} d^{-1} (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.802.0 d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime τ = 2.8–7.2 d for the gas phase reaction with OH radical (Kwok et al. 1995);

first-order photodegradation k = 0.98 h^{-1} with $t_{½}$ = 0.71 h when loaded on TiO_2 film under UV (λ > 300 nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: sunlight induced photolysis $t_{½}$ = 380 min in isooctane min and $t_{½}$ = 65 h dispersed as solid films (Buser 1988).

Groundwater:

Sediment: degradation $t_{½}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{½}$ = 10–100 yr (estimated, Suzuki et al. 2000).

Biota: mean $t_{½}$ ~43 d in rainbow trout (Niimi 1986);

biological $t_{½}$ = 43 d in rainbow trout (Niimi & Oliver 1986);

biological $t_{½}$ = 5–14 d in trout (Niimi 1987);

$t_{½}$ < 0.3 d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993)

TABLE 8.1.1.10.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4-tetrachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Shiu et al. 1988		Doucette & Andren 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		generator column-GC/ECD		gas saturation-GC/ECD		generator column-GC/ECD	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OA}
5	0.00034	4	0.00011	25	6.4 × 10^{-6}	0	11.131
15	0.00045	25	0.00047	50	2.6 × 10^{-4}	10	10.400
25	0.00063	40	0.00117	75	6.2 × 10^{-3}	20	9.896
35	0.00114			100	9.2 × 10^{-2}	30	9.455
45	0.002085			125	1.1	40	9.057
		ΔH_{sol}/(kJ mol^{-1}) = 46.8				25	9.70
		4–40 °C		ΔH_V/(kJ mol^{-1}) = 85.6			
ΔH_{sol}/(kJ mol^{-1}) = 33.36				ΔH_{subl}/(kJ mol^{-1}) = 118.53		log K_{OA} = a + b/(T/K)	
5–45 °C				ΔH_{fus}/(kJ mol^{-1}) = 31.2		a	–4.96
				ΔS_{fus}/(J mol^{-1} K^{-1}) = 68		b	4370
						enthalpy of phase change	
						ΔH_{OA}/(kJ mol^{-1}) = 83.60	

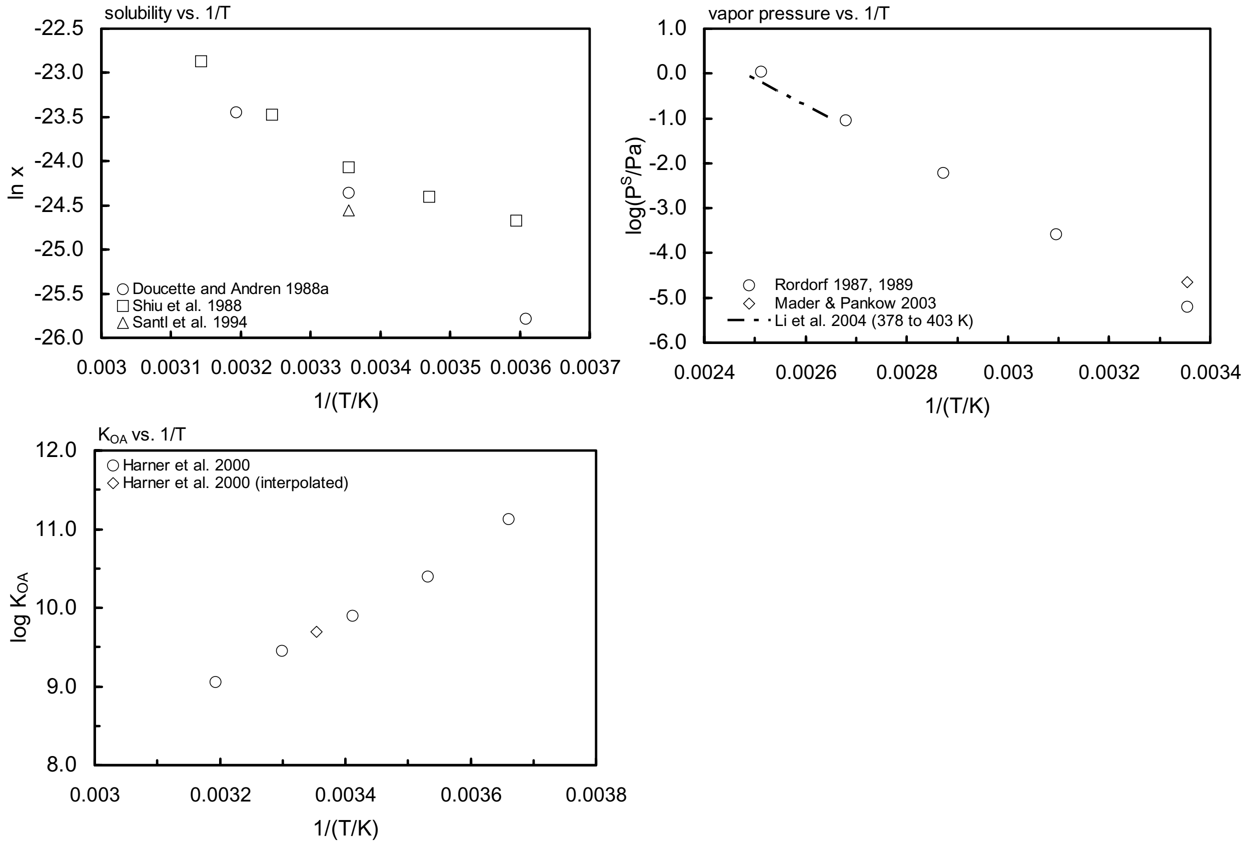
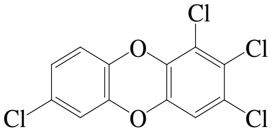


FIGURE 8.1.1.10.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4-tetrachlorodibenzo-*p*-dioxin.

8.1.1.11 1,2,3,7-Tetrachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,7-Tetrachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,7-TCDD
Chemical Name: 1,2,3,7-tetrachlorodibenzo-*p*-dioxin
CAS Registry No: 67028–18–6
Molecular Formula: $ClC_6H_3O_2C_6HCl_3$
Molecular Weight: 321.971
Melting Point (°C):
172–175 (Friesen et al. 1985)
Boiling Point (°C):
438.3 (calculated, Rordorf 1987, 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
186.52 (calculated-liquid density, Govers et al. 1990)
260.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
90.9 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
129.41 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
25.31 (Friesen & Webster 1990)
Entropy of Fusion, ΔS_{fus} (J/mol K):
82 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 0.0361 (mp at 172°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00042* (20°C, ^{14}C labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)
0.00043* (20°C, generator column-HPLC/LSC, measured range 20–40°C, Webster et al. 1985)
0.00028 (20°C, ^{14}C labeled, generator column-HPLC/LSC, Webster et al. 1986)
0.00048* (21°C, ^{14}C-labeled, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)
0.0161; 0.0131 (supercooled liquid S_L, GC-RI correlation, method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.0×10^{-6}* (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1986,1989)
7.0×10^{-6} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
5.0×10^{-6} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
2.69×10^{-5} (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)
$\log (P_L/\text{mmHg}) = 46.64 - 6978/(T/K) - 11.503 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.77 (calculated-P/C, Shiu et al. 1988)
1.78 (calculated-SOFA model, Govers & Krop 1998)
1.15; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

8.19, 8.59, 8.81; 8.22, 8.60, 8,81 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
8.18, 8.60 (HPLC-RT correlation, Sarna et al. 1984)
8.15, 7.58; 8.19, 7.72 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
6.91 (HPLC-RT correlation, Burkhard & Kuehl 1986)
6.48 (shake flask/slow stirring method-GC/ECD, mixture from fly-ash extract, Sijm et al. 1989a)
8.22 (recommended, Sangster 1993)
8.22 (recommended, Hansch et al. 1995)
7.05 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

3.17 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
3.44 (fathead minnow, steady-state, wet weight, Muir et al. 1985)
3.44, 4.44 (fathead minnow, wet wt. based, lipid based, Gobas & Schrap 1990)
3.17, 4.17 (rainbow trout, wet wt. based, lipid based, Gobas & Schrap 1990)
3.18, 2.90 (rainbow trout, Opperhuizen & Sijm 1990)
3.30, 3.38 (fathead minnow, Opperhuizen & Sijm 1990)
3.09, 3.02–3.14; 3.35, 3.30–3.37 (rainbow trout, range; fathead minnow, range, De Voogt et al. 1990)
5.50 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

4.26 (DOC, Muir et al. 1985)
5.39, 5.45, 5.59 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986)
5.98, 5.97, 5.91 (20, 30, 40°C, humic acid from peat bog, Webster et al. 1986)
6.55, 6.32, 6.44 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986)
7.87 (sediment/water., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 563 min for solution photolysis in n-hexadecane at 1.0 m from a GE Model RS sunlamp and $t_{½}$ = 156 min for surface photolysis on a clean soft glass surface under the same conditions (Nestrick et al. 1980);

first order $k = 18.13 \times 10^{-6}\ s^{-1}$ with $t_{½}$ = 10.69 h in water-acetonitrile (2:3 v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 33.52 \times 10^2\ d^{-1}$ with direct sunlight photolysis $t_{½}$ = 2.08 d in spring, $k = 39.41 \times 10^2\ d^{-1}$ with $t_{½}$ = 1.77 d in summer, $k = 21.77 \times 10^2\ d^{-1}$ with $t_{½}$ = 3.20 d in autumn, $k = 12.86 \times 10^2\ d^{-1}$ with $t_{½}$ = 8.73 d in winter, in aquatic bodies at latitude 40°N and $t_{½}$ = 8.73 d averaged over full year (Choudhary & Webster 1986, 1989).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is $4.73 \times 10^5\ L\ g^{-1}\ min^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = $(16–19) \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ at room temp. (Atkinson 1991)

k_{OH} = $(7.6–19) \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ and a calculated tropospheric lifetime of 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = $(2.0–5.1) \times 10^{-12}\ cm^3\ molecule^{-1}\ s^{-1}$ with a calculated tropospheric lifetime of 2.8–7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation: rate constant $k = 0.096\ d^{-1}$ for rainbow trout (Sijm et al. 1990).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 317\ d^{-1}$; $k_2 = 0.26\ d^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

k_1 = 529 d^{-1}; k_2 = 0.25 d^{-1} (fathead minnow, flow-through system, Muir et al. 1985)
k_2 = 0.178, 0.163 d^{-1} (rainbow trout, fathead minnow exposed to dioxins in their diets, Muir & Yarechewski 1988; quoted, Opperhuizen & Sijm 1990; Sijm et al. 1990)
k_1 = 420 to 213 mL g^{-1} d^{-1}; k_2 = 0.278 to 0.250 d^{-1} (rainbow trout exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
k_1 = 650 to 408 mL g^{-1} d^{-1}; k_2 = 0.322 to 0.170 d^{-1} (fathead minnow exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
k_2 = 9.5×10^{-2}, 19.1×10^{-2} d^{-1} (metabolic inhibitor PBO-treated rainbow trout, control fish, 2–21 d exposure: Sijm et al. 1990)
k_1 = 35 L kg^{-1} d^{-1}; $k_2 > 0.23$ d^{-1} (metabolic inhibitor PBO-treated goldfish after 120-h exposure, Sijm et al. 1993)
k_1 = 66 L kg^{-1} d^{-1}, 104 L kg^{-1} d^{-1} (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radical to be 0.8–2.0 d (Atkinson 1991); calculated tropospheric lifetime was 2.8–7.2 d for the gas-phase reaction with OH radical (Kwok et al. 1995).
Surface water: direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2}$ = 2.08 d in spring, $t_{1/2}$ = 1.77 d in summer, $t_{1/2}$ = 3.20 d in fall, $t_{1/2}$ = 5.42 d in winter, and $t_{1/2}$ = 8.73 d averaged over a full year (Choudhary & Webster 1986);
$t_{1/2}$ = 10.69 h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude: $t_{1/2}$ = 2.1 d in spring, $t_{1/2}$ = 1.8 d in summer, $t_{1/2}$ = 3.2 d in fall and $t_{1/2}$ = 5.4 d in winter (Choudhary & Webster 1986).
Groundwater:
Sediment: degradation $t_{1/2}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000).
Soil: degradation $t_{1/2}$ = 10–100 yr (estimated, Suzuki et al. 2000).
Biota: elimination $t_{1/2}$ = 2.7 d (Adams et al. 1986);
$t_{1/2}$ = 4 d in whole body of rainbow trout (Muir & Yarechewski 1988);
$t_{1/2}$ < 0.3 d for PBO treated gold fish in 120-h exposure studies (Sijm et al. 1993).

TABLE 8.1.1.11.1
Reported aqueous solubilities and vapor pressures of 1,2,3,7-tetrachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility						Vapor pressure	
Webster et al. 1985		Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989	
generator column-HPLC/LSC		generator column-GC/ECD		gen. col.-HLPC/LSC		vapor pressure correlation	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa
20	4.30×10^{-4}	20	4.30×10^{-4}	7.0	2.43×10^{-4}	25	1.0×10^{-6}
40	1.27×10^{-3}	40	1.27×10^{-3}	11.5	2.61×10^{-4}	50	5.9×10^{-5}
				17	4.03×10^{-4}	75	1.9×10^{-3}
ΔH_{sol}/(kJ mol^{-1}) = 50.68				21	4.80×10^{-4}	100	3.7×10^{-2}
25 °C				26	7.28×10^{-4}	125	0.57
				41	1.39×10^{-3}		
						ΔH_V/(kJ mol^{-1}) = 90.9	
				ΔH_{sol}/(kJ mol^{-1}) = 39.8		ΔH_{subl}/(kJ mol^{-1}) = 129.41	
				25 °C		ΔH_{fus}/(kJ mol^{-1}) = 36.6	
						ΔS_{fus}/(J mol^{-1} K^{-1}) = 82	

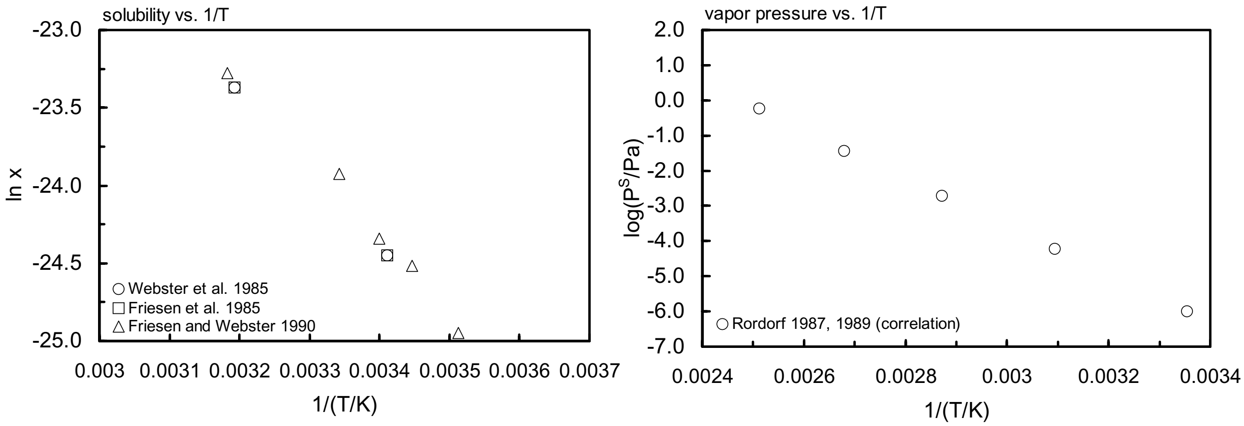
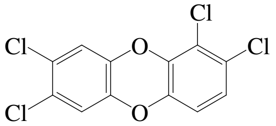


FIGURE 8.1.1.11.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,3,7-tetrachlorodibenzo-*p*-dioxin.

8.1.1.12 1,2,7,8-Tetrachlorodibenzo-*p*-dioxin



Common Name: 1,2,7,8-Tetrachlorodibenzo-*p*-dioxin
Synonym:1,2,7,8-TCDD
Chemical Name: 1,2,7,8-tetrachlorodibenzo-*p*-dioxin
CAS Registry No: 34816–53–0
Molecular Formula: $Cl_2C_6H_2O_2C_6H_2Cl_2$
Molecular Weight: 321.971
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

186.88	(calculated-liquid density, Govers et al. 1990)
260.6	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.00908 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
00223, 0.00908 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):

4.37×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
4.17×10^{-5}; 4.37×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
$\log (P_L/\text{mmHg}) = 46.50 - 6956/(T/K) - 11.503 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C):

1.48	(calculated-SOFA model, Govers & Krop 1998)
1.29; 1.48	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

6.38	(shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989a)
6.99	(calculated-SOFA model, Govers & Krop 1998)
6.93; 6.99	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.35, 6.30, 6.30, 6.44 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

5.51	(lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

7.99	(sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: solution photolysis $t_{½}$ = 491 min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{½}$ = 350 min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is 4.73×10^5 L g^{-1} min^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = 7.6×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (7.6–19) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^6 molecule/cm^3 (Atkinson 1991)

k_{OH}(calc) = (2.0–5.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 2.8–7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 38 L kg^{-1} d^{-1}; 49 L kg^{-1} d^{-1}; k_2 >0.9 d^{-1}; > 0.3 d^{-1} (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 66 L kg^{-1} d^{-1}, 104 L kg^{-1} d^{-1} (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.8–2.0 d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric lifetime τ(calc) = 2.8–7.2 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

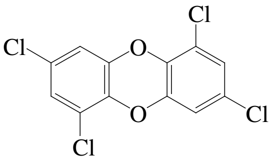
Groundwater:

Sediment: degradation $t_{½}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{½}$ = 10–100 yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{½}$ <0.7 d for PBO treated and $t_{½}$ <2.1 d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.13 1,3,6,8-Tetrachlorodibenzo-*p*-dioxin



Common Name: 1,3,6,8-Tetrachlorodibenzo-*p*-dioxin
Synonym: 1,3,6,8-TCDD
Chemical Name: 1,3,6,8-tetrachlorodibenzo-*p*-dioxin
CAS Registry No: 33423-92-6
Molecular Formula: $Cl_2C_6H_2O_2C_6H_2Cl_2$
Molecular Weight: 321.971
Melting Point (°C):
219–219.5 (Pohland & Yang 1972; Rordorf 1987,1989; Delle Site 1997)
Boiling Point (°C):
438.3 (calculated, Rordorf 1987, 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
192.34 (calculated-liquid density, Govers et al. 1990)
260.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
86.5 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
125.793 (Rordorf 1987)
118.6 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
74 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 0.0125 (mp at 219°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00032* (20°C, ^{14}C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Webster et al. 1985)
0.000317* (20°C, ^{14}C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)
0.000283, 0.000326, 0.000366, 0.000328 (^{14}C-labeled/LSC, Milli-Q treated water, lake water, simulated lake water, Milli-Q water, Servos & Muir 1989a)
0.0322 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.000537* (20°C, gas saturation, measured range 20–100°C, Webster et al. 1985)
7.0×10^{-7}* (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1986,1987,1989)
6.76×10^{-5} (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)
$\log (P_L/\text{mmHg}) = 46.99 - 6976/(T/K) - 11.503 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
$\ln (P/\text{Pa}) = 36.564 - 15127/(T/K)$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
$\ln (P/\text{Pa}) = (35.818 \pm 0.968) - (14262 \pm 380)/(T/K)$, temp range 378–408 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):
6.90 (23°C, batch stripping, Webster et al. 1985)
3.77 (calculated-P/C, Shiu et al. 1988)
1.15 (calculated-SOFA model, Govers & Krop 1998)

1.48; 1.15 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

8.72, 9.00, 9.42; 8.72, 9.02, 9.43 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
8.70, 9.02 (HPLC-RT correlation, Sarna et al. 1984)
8.70, 8.08; 8.70. 8.12 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
7.20, 7.13 (HPLC-RT correlation, Burkhard & Kuehl 1986)
7.13 (corrected HPLC-RT value, Burkhard & Kuehl 1986)
6.29 (shake flask/slow stirring method-GC/MS, Sijm et al. 1989a)
7.18 (recommended, Sangster 1993)
6.29 (recommended, Hansch et al. 1995)
6.79 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

3.03, 2.67 (fathead minnow, rainbow trout, Corbet et al. 1983, 1988)
3.39 (rainbow trout, steady-state, wet weight basis, Muir et al. 1985)
3.83 (fathead minnow, steady-state, wet weight basis, Muir et al. 1985)
3.39, 3.83 (rainbow trout average, fathead minnow average, Muir et al. 1986)
3.39, 3.32, 3.57 (*Oncorhynchus mykiss*, Servos et al. 1989)
1.08–3.75, 2.14, 1.76–1.93 (Amphipod in lake water, in simulated lake water, in water with Aldrich humic acid, Servos & Muir 1989a)
4.20, 4,20 (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)
5.00 (goldfish after 6 d exposure: metabolic inhibitor PBO-treated, Sijm et al. 1989b)
3.76, 3.54–3.90; 3.32, 3.23–3.40 (fathead minnow, range; rainbow trout, range, De Voogt et al. 1990)
3.83, 4.83 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
3.39, 4.39 (rainbow trout, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
3.46, 3.30, 3.15 (quoted, rainbow trout exposed to different concentrations, Opperhuizen & Sijm 1990)
3.76, 3.75 (fathead minnow exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
3.70 (10.1 ng/L for 0–10 d, predicted for biota held in lake enclosures, Servos et al. 1992b)
3.12 (17.7 ng/L for 0–10 d, invertebrates, Servos et al. 1992b)
3.20 (21.4 ng/L for 0–10 d, unionid clams & white suckers gill, Servos et al. 1992b)
2.36 (3.1 ng/L for 0–10 d, white suckers carcass, Servos et al. 1992b)
3.21 (1.6 ng/L for 14–24 d, invertebrates, Servos et al. 1992b)
2.95 (0.9 ng/L for 14–24 d, unionid clams, Servos et al. 1992b)
3.32 (2.1 ng/L for 14–24 d, white suckers gill, Servos et al. 1992b)
2.70 (1.0 ng/L for 14–24 d, white suckers carcass, Servos et al. 1992b)
4.54 (3.5 ng/L for 0–104 d, white suckers gill, Servos et al. 1992b)
4.26 (1.8 ng/L for 0–104 d, white suckers carcass, Servos et al. 1992b)
3.13 (gold fish, PBO-treated, 120-h exposure, Sijm et a1. 1993)
5.53 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

4.36 (DOC, De Voogt et al. 1990)
6.74 (calculated-K_{OW}, Corbet et al. 1988)
2.11–3.75, 2,39, 2.05–2.38 (DOC partition coeff., lake water, simulated lake water, Aldrich humic acid, Servos & Muir 1989a)
5.98–6.23 (sediment, Servos & Muir 1989b)
7.50 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.23 (derived from soot-water distribution coeff., Bärring et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$, or Lifetimes, τ:

Volatilization: 3.9 d in water of 0.5 m depth in a small pond (Corbet et al. 1988)

Photolysis: solution photolysis $t_{1/2}$ = 507 min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis on a clean glass surface under the same conditions with $t_{1/2}$ = 264 min (Nestrick et al. 1980; quoted, Muto et al. 1991);

first-order k = 59.57 × 10^{-6} s^{-1} in water-acetonitrile (2:3, v/v) at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2}$ = 0.35 d in spring, $t_{1/2}$ = 0.31 d in summer, $t_{1/2}$ = 0.53 d in fall, $t_{1/2}$ = 0.84 d in winter and $t_{1/2}$ = 1.47 d averaged over full year (Choudhary & Webster 1986; quoted, Muto et al. 1991)

$t_{1/2}$ = 14.0–28.5 h in outdoor pool and $t_{1/2}$ = 6.3–8.0 d in natural water in a Pyrex flask under sunlight (Corbet et al. 1988)

$t_{1/2}$ = 25 h in water column (Corbet et al. 1983)

$t_{1/2}$ = 6.3–8.0 d for natural water under sunlight and photodegradation $t_{1/2}$ = 0.3 d in summer sunlight at 40°N and $t_{1/2}$ = 7 d in a 1-L flask (Corbet et al. 1988)

photolysis k = 59.57 × 10^{-6} s^{-1} with $t_{1/2}$ = 3.24 h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: k = 198.13 × 10^{2} d^{-1} with $t_{1/2}$ = 0.35 d in spring, k = 226.99 × 10^{2} d^{-1} with $t_{1/2}$ = 0.31 d in summer, k = 130.91 × 10^{2} d^{-1} with $t_{1/2}$ = 0.53 d in fall, k = 82.85 × 10^{2} d^{-1} with $t_{1/2}$ = 0.84 d in winter; while experimentally determined sunlight photolysis $t_{1/2}$ = 3.5 d for ^{14}C labeled 1,3,6,8-TCDD in pond water (Choudhary & Webster 1989)

$t_{1/2}$ = 78.8 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation may be an important path of transformation (Corbet et al. 1988)

k (oxidative degradation rate of water dissolved PCDD by ozone) is 3.21 × 10^{5} L g^{-1} min^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = (16–19) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (7.6–19) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5 × 10^{6} molecule cm^{-3} at room temp. (Atkinson 1991)

k_{OH}(calc) = (2.0–5.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 2.8–7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 184 d^{-1}; k_2 = 0.10 d^{-1} (rainbow trout, flow-through system, Muir et al. 1985)

k_1 = 574 d^{-1}; k_2 = 0.10 d^{-1} (fathead minnow, Muir et al. 1985; quoted, Adams et al. 1986)

k_1 = 225, 221, 106 d^{-1} (rainbow trout fry, exposed to concn of 4, 74, 211 ng/L, 5-d uptake study, Muir et al. 1986)

k_2 = 0.074, 0.110, 0.111 d^{-1} (rainbow trout fry, exposed to 4, 74, 211 ng/L, 24 to 48-d depuration study, Muir et al. 1986)

k_1 = 526, 621 d^{-1} (fathead minnow, exposed to concn of 10, 41 ng/L, 5-d uptake study, Muir et al. 1986)

k_2 = 0.08, 0.122 d^{-1} (fathead minnow, exposed to concn of 10, 41 ng/L, 24 to 48-d depuration study, Muir et al. 1986)

k_1 = 225, 97 L kg^{-1} d^{-1} (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)

k_2 = 0.211 d^{-1} (fathead minnow, calculated, Corbet et al. 1983; quoted, Opperhuizen & Sijm 1990)

k_2 = 0.158 d^{-1} (rainbow trout, calculated, Corbet et al. 1983; quoted, Opperhuizen & Sijm 1990)

k_1 = 225, 221, 106 mL g^{-1}·d^{-1}; k_2 = 0.074, 0.110, 0.110 d^{-1} (rainbow trout exposed to different concentrations in a flow system, quoted, Opperhuizen & Sijm 1990)

k_1 = 526, 621 mL g^{-1}·d^{-1}; k_2 = 0.080, 0.122 d^{-1} (fathead minnow exposed to different concentrations in a flow system, quoted, Opperhuizen & Sijm 1990)

k_1 = 1200 d^{-1}; k_2 = 0.06 d^{-1} (filter-feeder, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

k_1 = 285 d^{-1}; k_2 = 0.12 d^{-1} (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

k_1 = 142, 116 L kg^{-1} d^{-1}; k_2 = 0.14, > 0.24 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
k_1 = 66 L kg^{-1} d^{-1}, 104 L kg^{-1} d^{-1} (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:
Air: tropospheric lifetime τ = 0.8–2.0 d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction rate with OH radicals (Atkinson 1991);
calculated tropospheric lifetime τ = 2.8–7.2 d for with OH radical (Kwok et al. 1995).
Surface water: direct sunlight photolysis in aquatic bodies at latitude 40°N for various seasons with half-lives: 0.35 d in spring, 0.31 d in summer, 0.53 d in fall, 0.84 d in winter and 1.47 d averaged over full year (Choudhary & Webster 1986);
$t_{1/2}$ = 14.0–28.5 h for outdoor pool and $t_{1/2}$ = 6.3–8.0 d for natural water in a Pyrex flask under sunlight (Corbet et al. 1988);
$t_{1/2}$ = 3.24 h for photolysis in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude calculated to be: $t_{1/2}$ = 0.35 d in spring, $t_{1/2}$ = 0.31 d in summer, $t_{1/2}$ = 0.53 d in fall, and $t_{1/2}$ = 0.84 d in winter (Choudhary & Webster 1989);
calculated transformation rate constant in simulated lake enclosure of 9.4×10^{-2} h^{-1} (Servos et al. 1992a).
Groundwater:
Sediment: $t_{1/2}$ = 51.2–69.2 d (Corbet et al. 1988);
calculated $t_{1/2}$ = 10 yr with a transformation rate constant k = 7.9×10^{-6} h^{-1} (Servos et al. 1992a);
degradation $t_{1/2}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000).
Soil: degradation $t_{1/2}$ = 10–100 yr (estimated, Suzuki et al. 2000).
Biota: $t_{1/2}$ = 4 d in rainbow trout (Neely 1979; quoted, Niimi & Oliver, 1983,1986);
$t_{1/2}$ = 4 d in rainbow trout (Corbet et al. 1983; quoted, Niimi & Oliver 1986);
$t_{1/2}$ = 2 d in rainbow trout (Muir et al. 1984);
$t_{1/2}$ = 6–9 d for both rainbow trout fry and fathead minnow (Muir et al. 1986);
$t_{1/2}$ = 6.90 d in fathead minnow (Adams et al. 1986);
$t_{1/2}$ = 41 to 44 d in rooted vegetable (Corbet et al. 1988);
$t_{1/2}$ = 15 d in whole body of rainbow trout (Muir et al. 1990);
half-lives in gold fish: $t_{1/2}$ = 4.8 d for PBO treated and $t_{1/2}$ < 0.3 d for control fish in 120-h exposure studies (Sijm et al. 1993)

TABLE 8.1.1.13.1
Reported aqueous solubilities and vapor pressures of 1,3,6,8-tetrachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure			
Webster et al. 1985		Friesen et al. 1985		Webster et al. 1985		Rordorf 1987, 1989	
generator column-HPLC/LSC		generator column-GC/ECD		gas saturation-GC		vapor pressure correlation	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
20	3.20×10^{-4}	20	3.20×10^{-4}	20	5.37×10^{-4}	25	7.0×10^{-7}
40	3.90×10^{-3}	40	3.90×10^{-3}	50	1.32×10^{-3}	50	3.6×10^{-5}
				100	1.12×10^{-2}	75	1.0×10^{-3}
						100	1.9×10^{-2}
						125	0.24
						$\Delta H_V/(kJ\ mol^{-1})$ = 86.5	
						$\Delta H_{subl}/(kJ\ mol^{-1})$ = 125.794	
						$\Delta H_{fus}/(kJ\ mol^{-1})$ = 36.6	
						$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1})$ = 74	

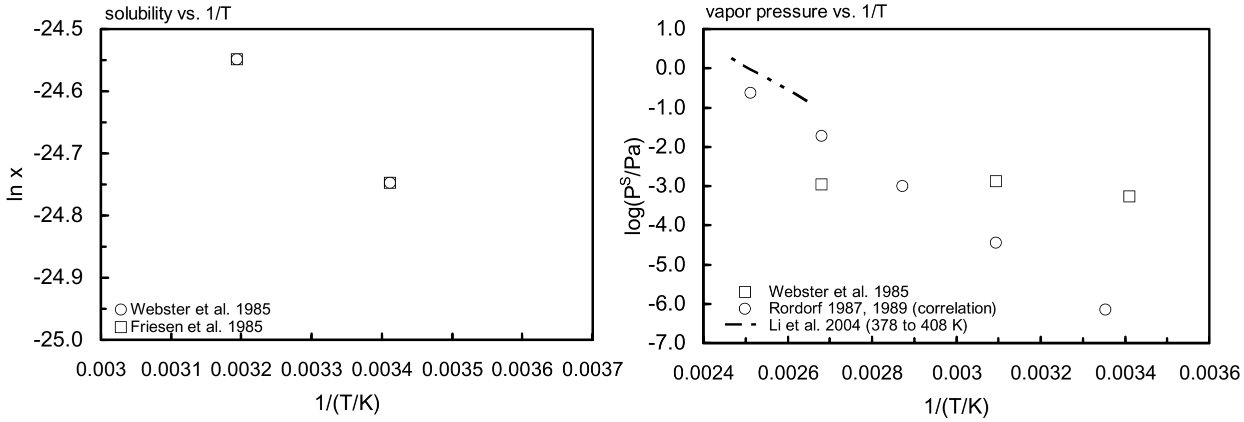
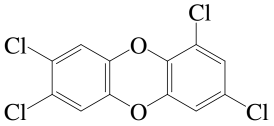


FIGURE 8.1.1.13.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,3,6,8-tetrachlorodibenzo-*p*-dioxin.

8.1.1.14 1,3,7,8-Tetrachlorodibenzo-*p*-dioxin



Common Name: 1,3,7,8-Tetrachlorodibenzo-*p*-dioxin
Synonym:1,3,7,8-TCDD
Chemical Name: 1,3,7,8-tetrachlorodibenzo-*p*-dioxin
CAS Registry No: 50585–46–1
Molecular Formula: $Cl_2C_6H_2O_2C_6H_2Cl_2$
Molecular Weight: 321.971
Melting Point (°C):
193.5–195 (Rordorf 1986, 1987, 1989)
Boiling Point (°C):
438.3 (calculated, Rordorf 1986,1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
188.33 (calculated-liquid density, Govers et al. 1990)
260.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
88.9 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
127.77 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
78 (Rordorf 1986, 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0203 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
00223, 0.0203 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
8.4×10^{-7}, 4.5×10^{-5}, 1.4×10^{-3}, 2.6×10^{-2}, 0.35 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
8.32×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
4.17×10^{-5}; 8.32×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
$\log (P_L/\text{mmHg}) = 46.80 - 6977/(T/K) - 11.503 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C):
1.26 (calculated-SOFA model, Govers & Krop 1998)
1.29; 1.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.80 (calculated-SOFA model, Govers & Krop 1998)
6.93; 6.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
6.30; 6.29, 6.28, 6.40, 6.44 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

5.52 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

7.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: solution photolysis $t_{½}$ = 153 min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{½}$ = 160 min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

$t_{½}$ = 86.6 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 13×10^{-12} cm^3 $molecule^{-1}·s^{1}$ at room temp. (Atkinson 1991)

k_{OH} = $(7.6 - 19) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^6 molecule cm^{-3} at room temp. (Atkinson 1991)

k_{OH}(calc) = $(2.0 - 5.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 2.8–7.2 d at for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:.

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 57 L kg^{-1} d^{-1}; 99 L kg^{-1} d^{-1}; k_2 = 0.14 d^{-1}; > 0.24 d^{-1} (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 66 L kg^{-1} d^{-1}, 104 L kg^{-1} d^{-1} (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.8–2.0 d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime τ = 2.8–7.2 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

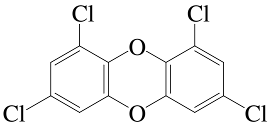
Groundwater:

Sediment: degradation $t_{½}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{½}$ = 10–100 yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{½}$ = 2.1 d for PBO treated and $t_{½}$ < 0.4 d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.15 1,3,7,9-Tetrachlorodibenzo-*p*-dioxin



Common Name: 1,3,7,9-Tetrachlorodibenzo-*p*-dioxin
Synonym:1,3,7,9-TCDD
Chemical Name: 1,3,7,9-tetrachlorodibenzo-*p*-dioxin
CAS Registry No: 62470–53–5
Molecular Formula: $Cl_2C_6H_2O_2C_6H_2Cl_2$
Molecular Weight: 321.971
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
192.34 (calculated-liquid density, Govers et al. 1990)
260.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
123.6 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0294 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
00294, 0.0294 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
5.50×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
5.89×10^{-5}; 5.50×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
$\log (P_L/\text{mmHg}) = 46.86 - 6956/(T/K) - 11.503\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
$\ln (P/\text{Pa}) = (37.221 \pm 0.469) - (14864 \pm 185)/(T/K)$; temp range 383–408 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.589 (calculated-SOFA model, Govers & Krop 1998)
1.42; 0.589 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)
6.68 (calculated-SOFA model, Govers & Krop 1998)
6.83; 6.68 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
6.28, 6.12, 6.47, 6.44 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
5.67 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:
7.51 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: solution photolysis $t_{½}$ = 499 min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{½}$ = 169 min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

$t_{½}$ = 79.7 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (16 – 19) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (7.6 – 19) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5 × 10^6 molecule cm^{-3} at room temp. (Atkinson 1991)

k_{OH}(calc) = (2.0–5.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 2.8–7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 54 L kg^{-1} d^{-1}, 98 L kg^{-1} d^{-1}; k_2 <0.1 d^{-1}, >2.1 d^{-1} (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 66 L kg^{-1} d^{-1}, 104 L kg^{-1} d^{-1} (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime τ = 0.8–2.0 d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime τ = 2.8–7.2 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

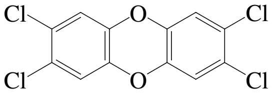
Groundwater:

Sediment: degradation $t_{½}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{½}$ = 10–100 yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{½}$ > 7 d for PBO treated and $t_{½}$ < 0.3 d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.16 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin



Common Name: 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin
Synonym: 2,3,6,7-tetrachlorodibenzo-*p*-dioxin, TCDD, TCDBD, 2,3,6,7- TCDD, 2,3,7,8-TCDD, dioxin
Chemical Name: 2,3,7,8-tetrachlorodibenzo-*p*-dioxin
CAS Registry No: 1746–01–6
Molecular Formula: $Cl_2C_6H_2O_2C_6H_2Cl_2$
Molecular Weight: 321.971
Melting Point (°C):
295 (Lide 2003)
Boiling Point (°C):
421.2 (Schroy et al. 1985a)
Density (g/cm^3 at 20°C):
1.827 (solid at 25°C, Boer et al. 1972; Schroy et al. 1985a)
1.021 (liquid at normal boiling point, Schroy et al. 1985a)
Molar Volume (cm^3/mol):
184.32, 184.97 (calculated-liquid density, crystalline volume, Govers et al. 1990)
188.34 (liquid molar volume, Govers et al. 1990)
260.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
71.71 (at normal bp, Schroy et al. 1985a)
79.9 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
123.91 (Schroy et al. 1985b)
124.001 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
38.91 (Boer et al. 1972; Schroy et al. 1985a,b; Ruelle & Kesselring 1997)
38.9, 36.6 (Obs., predicted, Rordorf 1986, 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
69 (Rordorf 1986, 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00244 (mp at 295°C)
0.0017 (Shiu et al. 1988)
4.07×10^{-4} (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0002 (shake flask-GC/ECD, Crummett & Stehl 1973)
3.17×10^{-4} (^{14}C-labeled, generator column-HPLC/LSC, Webster et al. 1983)
1.93×10^{-5} (shake flask-GC/MS, Marple et al. 1986a)
7.91×10^{-6} (^{14}C-labeled, Adams & Blaine 1986)
1.29×10^{-5}, 4.83×10^{-4} (4.3, 17.3°C, generator column-GC/MS, Lodge 1989)
$\log [S_L/(mol/L)] = 0.190–2089/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
0.0158 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.0×10^{-7} (^{14}C-gas saturation method, Jaber & Podoll 1983)
$(4.50 \pm 2) \times 10^{-6}$ (gas saturation-GC, Rordorf 1985a)
$(3.5–6.3) \times 10^{-6}$, $(1.3–3.1) \times 10^{-4}$, $(2.8–8.9) \times 10^{-2}$, $(3.9–15.9) \times 10^{-2}$, $(4.4–21.9) \times 10^{-1}$ (25, 50, 75, 100, 125°C, predicted using estimated ΔH_{sub} and ΔS_{sub} for tetra-chloro isomers, Rordorf 1985a)
4.61×10^{-7}* (30.1°C, gas saturation-GC/MS, measured range 30.1–71.1°C Schroy et al. 1985a,b)
$\log (P/mmHg) = 12.89784 – 6477.132/(273.15 + t/°C)$; temp range 10–305°C (Antoine eq., from gas saturation-GC/MS, Schroy et al. 1985b)

log (P/mmHg) = 8.78307 – 4098.173/(273.15 + t/°C); temp range 305–420°C (Antoine eq., from gas saturation-GC/MS, Schroy et al. 1985b)
2.02×10^{-7}*, 4.60×10^{-7}, 9.65×10^{-6}, 4.58×10^{-5}, 1.59×10^{-4} (25, 30, 50, 62, 71°C, results derived from Antoine eq., gas saturation-GC/MS, Schroy et al. 1985b)
ln (P/Pa) = 34.570834 – [14903.438/(T/K)], temp range: 283.15–578.15 K (gas saturation, Schroy et al. 1985a)
ln (P/Pa) = 25.104351 – 93430.391/(T/K), temp range: 578.15–703.15 K (gas saturation, Schroy et al. 1985a)
8.71×10^{-6}* (20°C, gas saturation-LSC, measured range 20–100°C, Webster et al. 1985)
9.87×10^{-8} (^{14}C-gas saturation, Podoll et al. 1986)
8.14×10^{-8}, 6.0×10^{-5} (20°C, quoted: solid P_S, supercooled liquid P_L, Bidleman & Foreman 1987)
2.0×10^{-7}* (gas saturation-GC, measured range 25–125°C, Rordorf 1987, 1989)
6.20×10^{-7}, 2.6×10^{-5}, 6.1×10^{-4}, 9.7×10^{-3}, 1.1×10^{-1} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1987, 1989)
6.17×10^{-4}; 2.51×10^{-7} (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 12.66–5739/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 9.05–3663/(T/K) (supercooled liquid, Passivirta et al. 1999)
1.17×10^{-4}; 5.75×10^{-5} (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
log (P_S/Pa) = 15.0391 – 6482.7/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
5.25×10^{-4} (supercooled liquid P_L, Harner et al. 2000)
2.57×10^{-5}; 5.75×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
5.56×10^{-7} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
3.35×10^{-4} (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
log (P_L/mmHg) = 49.89 – 6705/(T/K) – 12.569·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C and reported temperature dependence equations):
0.0021 (calculated-P/C, Mabey et al. 1982)
0.152 (calculated-P/C, Crosby 1985)
0.212 (calculated-P/C, Schroy et al. 1985)
1.64 (calculated-P/C, Podoll et al. 1986)
1.63, 3.34, 10.34 (calculated-P/C, Shiu et al. 1988)
7.93 (calculated-P/C, Jury et al. 1990)
1.62 (calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa m^3/mol)] = 8.86–1574/(T/K) (Passivirta et al. 1999)
1.12; 1.62 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
5.38 (Crummett & Stehl 1973)
6.19 (Neely 1979; Veith et al. 1979; Corbet et al. 1983)
6.15 (Kenaga 1980;)
8.93 (HPLC-RT correlation, Sarna et al. 1984)
7.02 (HPLC-RT correlation, Burkhard & Kuehl 1986)
6.64 (shake flask-GC/MS, Marple et al. 1986b)
6.42 (shake flask/slow stirring method-GC/MS, Sijm et al. 1989a)
7.02 (recommended, Sangster 1993)
6.53 (recommended, Hansch et al. 1995)
7.06 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
9.70 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
10.05*; 9.91 (generator column-GC; calculated, Harner et al. 2000)
11.04 (7°C, GC-retention time correlation, Harner et al. 2000)
log K_{OA} = –6.19 + 4840/(T/K); temp range 10–50°C (generator column-GC/ECD, Harner et al. 2000)
9.95 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:

1.69, 2.34, 2.08 (*daphnia*, ostracod, brine shrimp, ^{14}C-labeled-LSC, Matsumura & Benezet 1973)
4.30–4.41; 3.6–3.95 (snail, *gambusia*, *daphnids*; duckweed, algae, catfish; Isensee & Jones 1975)
3.96 (rainbow trout, Branson et al. 1985)
3.90 (fathead minnow, steady-state, wet weight, Adams et al. 1986)
3.73, 4.55 (fish: flowing water test, static ecosystem test, Kenaga & Goring 1980, Kenaga 1980)
3.97 (rainbow trout, Branson et al. 1983)
3.97, 3.67 (rainbow trout: whole body, muscle, Branson et al. 1985)
1.38–1.60 (rhesus monkey, Geyer et al. 1986)
4.11 (guppy, Opperhuizen et al. 1986)
4.43, 4.59 (rainbow trout: measured average, estimated BCF at steady-state, for 28-d exposure, Mehrle et al. 1988)
4.30, 5.0 (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)
3.89, 4.59 (fathead minnow, rainbow trout, De Voogt et al. 1990)
5.80, 5.90 (goldfish after 6 d exposure: PBO-treated, control, Sijm et al. 1989b)
4.11, 5.64 (guppy, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
3.97, 4.70; 4.97, 5.70 (rainbow trout, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
4.63, 4.40 (pine needle/air BCF values, Reissinger et al. 1989)
4.59, 4.58, 4.93, 4.57, 3.97 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
4.11, 3.90, 3.78 (guppy, fathead minnow, mosquito fish, quoted, Opperhuizen & Sijm 1990)
2.62 (human, Webster & Connett 1991)
5.24; 4.91 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
5.24; 4.83; 5.02 (guppies, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
5.24; 5.48 (lipid wt. base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
5.71, 6.71 (fish medeka 10% lipid: BCF_W, BCF_L, Geyer et al. 2000)
6.02, 6.05 (fish muscle log BCF_L calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

5.67 (organic carbon soil, calculated-K_{OW}, Kenaga 1980)
6.95, 7.39–7.58 (calculated-K_{OW}, 10 soils from Missouri & New Jersey, Jackson et al. 1985)
6.22–6.54; 5.96–6.09 (red clay soil from Missouri, Alluvial soil from Missouri, Marple et al. 1986)
4.83 (hydroxy aluminum-clay, Srinivasan & Fogler 1987)
6.60 (^{14}C-labeled, soil, batch equilibrium-sorption isotherm, GC/ECD, Walters & Guiseppi-Elie 1988)
3.06 (soil, Eduljee 1987)
6.30; 7.59; 7.25 (Lake Ontario sediment; solids; DOC dissolved organic carbon; batch equilibrium-sorption isotherm, Lodge & Cook 1989)
6.24, 6.10, 5.10 (Eglin Air Force Base soil/water with 0.01% surfactant from Florida at pH 4, 7, 8.5, batch equilibrium-GC, Puri et al. 1989)
6.50, 5.86, 4.81 (Time Beach soil/water with 0.01% surfactant from Missouri at pH 4, 7, 8.5, Puri et al. 1989)
5.70, 5.09, 4.76 (Visalia soil/water with 0.01% surfactant from California at pH 4, 7, 8.5, Puri et al. 1989)
6.44, 6.66 (batch equilibrium-sorption isotherms: 2-d, 10-d isotherm, regression analysis for sorption of uncontaminated Time Beach soil from water, Walters et al. 1989)
6.14 (soil, Jury et al. 1990)
6.80 (Baltic sea particulate filed samples, concn distribution-GC/MS, Broman et al. 1991)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: probably not an important process (Callahan et al. 1979)
$t_{½}$ = 20–200 d from water column which will be slowed down further by the fact that it is sorbed to the sediment and biota (Mill 1985)
$t_{½}$ ~32 d for ponds and $t_{½}$ ~16 d for rivers (Podoll et al. 1986)
$t_{½}$ = 104 d from soil by calculation assuming diffusion of TCDD in soil is vapor-dominated up to volumetric water content of 0.3 m^3/m^3, and then liquid-dominated to saturation (Eduljee 1987)
$t_{½}$ = 190 d (Thibodeaux & Lipsky 1985; quoted, Eduljee 1987)

$t_{1/2}$ = 365 d for volatilization from below surface soil (Jury et al. 1990)

k = 0.0054 h^{-1} with $t_{1/2}$ = 128 h from grass foliage (McCrady & Maggard 1993)

Photolysis:

stable to sunlight for at least 14 d in distilled water (Crosby et al. 1971; quoted, Dougherty et al. 1991)

$t_{1/2}$ = 3 h in methanol solution in sunlight (Plimmer et al. 1973)

$t_{1/2}$ = 56 min for vapor in sunlight (Peterson 1976; quoted, Mill 1985)

thin film of TCDD on glass plates showed transformation at about 6 h (Crosby & Wong 1977);

$t_{1/2}$(soln) = 56.8 min in *n*-hexadecane on a clean soft glass surface at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2}$ = 140 h on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984; Dougherty et al. 1991)

TCDD extracted from the aqueous sludge with hexane can be continuously degraded by a mercury arc of UV radiation (Exner et al. 1982; quoted, Crosby 1985)

$t_{1/2}$ ~ 1d in water, $t_{1/2}$ = 0.1 d in vapor and $t_{1/2}$ = 1–100 d in soil with $t_{1/2}$ = 50 d for a small fraction in water column in equilibrium with sediment sorbed with TCDD (Mill 1985)

$k_P = 6.94 \times 10^{-6}$ s^{-1} with $t_{1/2}$ = 27 h in a 90:10 mixture of distilled water and acetonitrile under summer sunlight; k_P = 0.15 d^{-1} with $t_{1/2}$ = 6 d in summer sunlight at 40°L surface waters (Dulin et al. 1986)

$t_{1/2}$ = 81 h after adjusting for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)

k = 0.14 d^{-1} with $t_{1/2}$ = 118 h in winter, k = 0.61 d^{-1} with $t_{1/2}$ = 27 h in spring, k = 0.78 d^{-1} with $t_{1/2}$ =21 h in summer, and k = 0.32 d^{-1} with $t_{1/2}$ = 51 h in autumn for aqueous dissolved TCDD in sunlight over four seasons at 40°N latitude (Podoll et al. 1986)

photodegradation $t_{1/2}$ = 10 min, a very rapid process at soil surface during the day (Facchetti et al. 1986)

$t_{1/2}$ = 14 min sunlight induced photolysis in isooctane solution and sunlight induced solid phase $t_{1/2}$ = 300 h dispersed as solid films (Buser 1988)

k = 5.9×10^{-3} s^{-1} rate constant for photolysis in air at 150–350°C (Orth et al. 1989)

k = 0.15 min^{-1} first-order photolysis rate constant in isooctane and over 90% was lost in 21 min of irradiation in isooctane whereas only greater than 55% TCDD remained in soil after 15 d of irradiation (Kieatiwong et al. 1990)

photolytic degradation $t_{1/2}$ = 4.5 h in extract from fly ash exposed to UV light from a distance of 20 cm for native congener and $t_{1/2}$ = 5.2 h for ^{13}C-labeled congener in tetradecane solution (Tysklind & Rappe 1991)

$t_{1/2}$ = 31 min in hexadecane and $t_{1/2}$ = 27 min in ethyl oleate (Dougherty et al. 1991)

photodegradation k = 0.0156 h^{-1} with $t_{1/2}$ = 44 h for TCDD sorbed to grass foliage and exposed to natural sunlight (McCrady & Maggard 1993)

$t_{1/2}$ = 52 h, direct sunlight photolysis in water-acetonitrile in midday of mid-summer at 40°N (quoted, Zepp 1991)

$t_{1/2}$ = 55.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k = 6×10^{-7} s^{-1} with $t_{1/2}$ = 320 h, estimated for the reaction with 3×10^{-15} mole OH radicals in vapor phase (Singh 1977; quoted, Mill 1985)

laboratory tests shown that 99.5% TCDD was oxidized in 21 s at 800°C while only 50% reacted at 700°C (Esposito et al. 1980; quoted, Crosby 1985)

$k_{OH} = 2 \times 10^{8}$ mol^{-1} s^{-1} with $t_{1/2}$ = 13 d for oxidation in vapor phase (Mill 1985)

$k_{OH} > 1.0 \times 10^{8}$ mol^{-1} s^{-1}, 1.7×10^{-13} cm^3 $molecule^{-1}$ s^{-1} with $t_{1/2}$ = 200 h (Podoll et al. 1986)

k_{OH}(calc) = 9×10^{-12} cm^3 $molecule^{-1}$ s^{-1} with an atmospheric lifetime τ ~ 3 d (Atkinson 1987a)

k_{OH}(calc) = 8.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship Atkinson 1987b)

photooxidation $t_{1/2}$ = 22.3–223 h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

k = 1.33×10^{5} L g^{-1} min^{-1}, the oxidative degradation of water dissolved TCDDs by ozone takes place only under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = 7.6×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (7.6 - 19) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^{6} molecule/cm^3 at room temp. (Atkinson 1991)

k_{OH-}(calc) = 4×10^{9} M^{-1} s^{-1} in aqueous solutions (Haag & Yao 1992)

k_{OH}(calc) = (2.0 - 5.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 2.8–7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis: hydrolysis is not likely under environmental conditions (Callahan et al. 1979; Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$t_{½}$(aq.aerobic) = 10032 h, based on soil die-away test data (Kearney et al. 1971; quoted, Howard et al. 1991) and $t_{½}$ = 14160 h, based on lake water and sediment dieaway test data (Ward & Matsumura 1978; quoted, Howard et al. 1991)

$t_{½}$ >1.0 yr (Callahan et al. 1979);

$t_{½}$(aq. anaerobic) = 40128–56640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: k = 1 × 10^{-10} mL $cell^{-1}$ h^{-1} for bacterial transformation in water (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 4.64 mL g^{-1} h^{-1}; k_2 = 5.00 × 10^{-4} h^{-1} (rainbow trout, Neely 1979)

k_1 = 108 mL g^{-1} d^{-1}; k_2 = 0.012 d^{-1} (rainbow trout, Branson et al. 1983,1985)

k_1 = 476 mL g^{-1} d^{-1}; k_2 = 0.120 d^{-1} (fathead minnow, Adams et al. 1986)

k_1 = 600 mL g^{-1} d^{-1}; k_2 = 0.046 d^{-1} (guppy, Opperhuizen et al. 1986)

k_1 = 1832, 1543, 1337, 1591 d^{-1} and k_2 = 0.047, 0.041, 0.015, 0.043 d^{-1} (rainbow trout, exposed to 38 pg/L, 176 pg/L, 382 pg/L, 702 pg/L for 28 d, Mehrle et al. 1988)

k_1 = 216, 604 L kg^{-1} d^{-1} (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)

k_2 = 0.008 d^{-1} (rainbow trout, quoted, Opperhuizen & Sijm 1990)

k_1 = 381 mL g^{-1} d^{-1}; k_2 = 0.048 d^{-1} (fathead minnow, quoted, Opperhuizen & Sijm 1990)

k_1 = 100 mL g^{-1} d^{-1} (mosquito fish, quoted, Opperhuizen & Sijm 1990)

k_1 = 86 L kg^{-1} d^{-1} (goldfish, 120-h exposure, metabolic inhibitor PBO-treated; Sijm et al. 1993)

k_1 = 66 L kg^{-1} d^{-1}, 104 L kg^{-1} d^{-1} (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 >1.3 d^{-1}; < 0.1 d^{-1} (goldfish after 120-h exposure: metabolic inhibitor PBO-treated; control, Sijm et al. 1993)

k_1 = 500 L kg^{-1} d^{-1}; k_2 = 0.049 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

k_2 = 0.0061 d^{-1} with a biological $t_{½}$ = 49 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

k_2 = 0.0246 d^{-1} with $t_{½}$ = 28 d (newly contaminated oysters, Gardinali et al. 2004)

k_2 = 0.0199 d^{-1} with $t_{½}$ = 35 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: dominant transformation process in the atmosphere (Atkinson et al. 1982)

$t_{½}$ = 200 h for reaction with OH radical (Podoll et al. 1986)

atmospheric lifetime of ~3 d at room temp. (Atkinson 1987a)

$t_{½}$ = 22.3–223 h, based on estimated photooxidation half-life in air (Howard et al. 1991)

$t_{½}$ = 1 h, an upper limit, undergo rapid photolysis in vapor phase (Travis & Hattemer-Frey 1987)

atmospheric k = 0.012 min^{-1} with $t_{½}$ = 58 min in summer sunlight at 40°N latitude (Buser 1988)

reaction rate constant k ~ 0.02 h^{-1} (Paterson et al. 1990)

tropospheric lifetime τ(calc) = 0.8–2.0 d for reaction with OH radical (Atkinson 1991)

tropospheric lifetime τ(calc) = 2.8–7.2 d for with OH radical (Kwok et al. 1995);

$t_{½}$ = 200 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis $t_{½}$ = 3 h in methanol solution under sunlight (Plimmer et al. 1973);

$t_{½}$ = 600 d in a model aquatic environment (Ward & Matsumura 1978);

reaction rate constant estimated to be 2.6 × 10^{-5} h^{-1} (Mackay et al. 1985);

calculated sunlight photolysis half-lives over four seasons at 40°N latitude averaged over for 24 h exposure per day: $t_{½}$ = 130 h in winter, $t_{½}$ = 28 h in spring, $t_{½}$ = 20 h in summer and $t_{½}$ = 52 h in fall (Mill et al. 1982; quoted, Mill 1985);

calculated photolysis half-lives in sunlight at 40°N latitude: $t_{½}$ = 118 h in winter, $t_{½}$ = 27 h in spring, $t_{½}$ = 21 h in summer and $t_{½}$ = 51 h in fall (Podoll et al. 1986);

photolysis $t_{½}$ = 40 h in near-surface waters is an important degradative pathway (Travis & Hattemer-Frey 1987);

$t_{½}$ = 14 min, sunlight-induced photolysis half-life in isooctane (Buser 1988);

reaction rate constant estimated to be 0.008 h^{-1} (Paterson et al. 1990);

photolysis $t_{1/2}$ = 27–81 h, aerobic $t_{1/2}$ = 1.15–1.62 yr, anaerobe $t_{1/2}$ = 4.58–6.45 yr (Howard et al. 1991)
$t_{1/2}$ = 4000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
Groundwater: $t_{1/2}$ = 20064–28320 h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).
Sediment: $t_{1/2}$ = 12000–14400 h in aquatic sediment (Ward & Matsumura 1978; quoted, Quensen & Matsumura 1983)
reaction rate constant k ~ 8.0×10^{-6} h^{-1} (Mackay et al. 1985)
k ~1.5×10^{-5} h^{-1} (Paterson et al. 1990)
$t_{1/2}$ >1 yr (O'Keefe et al. 1986)
$t_{1/2}$ = 9.9–98 yr (Geyer et al. 2000)
degradation $t_{1/2}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000)
$t_{1/2}$ = 900000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{1/2}$ = 10032–14160 h, based on soil dieaway test data for two soils (Howard et al. 1991);
$t_{1/2}$ ~ 1 yr (Kearney et al. 1973; quoted, Quensen & Matsumura 1983);
degradation $t_{1/2}$ = 10–12 yr in soil (De Dimenico et al. 1980, Kimbrough et al. 1984);
$t_{1/2}$ ~ 1 yr if applied to surface on soil with 2,4-D (Nash & Beall 1980);
k ~ 8.0×10^{-6} h^{-1} (Mackay et al. 1985)
k ~1.1×10^{-5} h^{-1} (Paterson et al. 1990)
$t_{1/2}$ = 10 min during the day, photodegradation is a rapid process at the soil surface (Facchetti et al. 1986);
$t_{1/2}$ ~ 10 yr in soil if TCDD is on or near the surface and $t_{1/2}$ = 100 yr if TCDD is buried at greater depth (Nauman & Schaum 1987)
calculated $t_{1/2}$ = 10 yr (Eduljee 1987)
$t_{1/2}$ = 10 yr or longer (Boddington et al. 1990)
$t_{1/2}$ = 365 d for volatilization to atmosphere below surface soil (Jury et al. 1990)
$t_{1/2}$ = 10 yr (Geyer et al. 2000)
degradation $t_{1/2}$ = 10–100 yr in soils (estimated, Suzuki et al. 2000)
$t_{1/2}$ = 900000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000)
Biota: $t_{1/2}$ = 31 d, estimated half-life in rat (Rose et al. 1976; quoted, Birnbaum 1985);
$t_{1/2}$ = 11 d, estimated half-life in hamster (Olsen et al. 1980; quoted, Birnbaum 1985)
$t_{1/2}$ = 30 d, estimated half-life in guinea pig (Decad et al. 1981a; quoted, Birnbaum 1985)
$t_{1/2}$ = 11–24 d, estimated half-life in mouse(Gasiewicz et al. 1983; quoted, Birnbaum 1985)
depuration $t_{1/2}$ = 58 d, total body burden of ^{14}C-TCDD in whole rainbow trout (Branson et al. 1983, 1985)
$t_{1/2}$ = 17–37 d in mouse, $t_{1/2}$ = 31 d in rat and $t_{1/2}$ = 30 d in guinea pig (quoted, Van den Berg et al. 1985)
elimination $t_{1/2}$ = 14.5 d from fathead minnow (Adams et al. 1986)
$t_{1/2}$ = 105 d in whole body of rainbow trout (Kleeman et al. 1986);
$t_{1/2}$ = 300–325 d in carp (Kuehl et al. 1986)
biological $t_{1/2}$ = 58 d for rainbow trout (Niimi & Oliver 1986)
$t_{1/2}$ – 5.8 yr in human (estimated, Poiger & Schlatter 1986)
$t_{1/2}$ >336 d for carps in Lake Superior (Kuehl et al. 1987)
$t_{1/2}$ – 6.7 yr in human (estimated, Kissel & Robarge 1988)
elimination $t_{1/2}$ = 15–48 d from rainbow trout for exposures of different concn (Mehrle et al. 1988)
$t_{1/2}$ – 7.1 yr in human (estimated, Pirkle et al. 1989; quoted, Webster & Connett 1991)
$t_{1/2}$ = 5 – 8 yr for human, $t_{1/2}$ = 17.4–31 d for rats, $t_{1/2}$ = 9.6–24.4 d for mice, $t_{1/2}$ = 22–93.7 d for guinea pigs, $t_{1/2}$ = 12.0–150 d for hamsters, $t_{1/2}$ = 1 yr for monkeys (Boddington et al. 1990)
$t_{1/2}$ = 40.3 d for lactating cows (Olling et al. 1991)
$t_{1/2}$ = 5 – 10 yr assumed half-life for human (Schecter & Ryan 1991)
elimination $t_{1/2}$ = 35–37 d from lake trout sac fry (Walker et al. 1991)
$t_{1/2}$ = 4.4 yr for a 70 kg non-lactating "reference" human (Webster & Connett 1991)
$t_{1/2}$ < 0.5 d for metabolic inhibitor PBO treated gold fish and $t_{1/2}$ > 7 d for control fish in 120-h exposure studies (Sijm et al. 1993)
elimination $t_{1/2}$ = 45 d from soft-shell clam (Brown et al. 1994)
biological $t_{1/2}$ = 49 d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994)
reported $t_{1/2}$ = 8–24.4 d for mice, $t_{1/2}$ = 30.2 and 93.7 d for guinea pigs, $t_{1/2}$ = 20–28.9 d for rats and $t_{1/2}$ = 365–3470 d for humans (Miniero et al. 2001).
depuration $t_{1/2}$ = 28 d for newly contaminated oysters, and $t_{1/2}$ = 35 d for chronically contaminated oysters (Gardinali et al. 2004)

TABLE 8.1.1.16.1
Reported vapor pressures of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin at various temperatures

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Schroy et al. 1985a		Schroy et al. 1985b		Webster et al. 1985		Rordorf 1987, 1989	
gas saturation		gas saturation		gas saturation-LSC		gas saturation-GC/ECD	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30.1	4.61×10^{-7}	30	4.67×10^{-7}	20	8.71×10^{-6}	25	2.0×10^{-7}
30.2	5.19×10^{-7}	54.6	1.83×10^{-5}	50	1.12×10^{-5}	50	9.5×10^{-6}
30.3	8.73×10^{-7}	62	4.97×10^{-5}	100	1.72×10^{-5}	75	2.6×10^{-4}
54.6	2.06×10^{-5}	71	1.59×10^{-4}			100	4.6×10^{-3}
55	1.37×10^{-5}					125	5.7×10^{-2}
55.2	1.94×10^{-5}	Antoine eq. for 10–305 °C					
61.9	3.71×10^{-5}	eq. 2	P/mmHg			ΔH_V/(kJ mol^{-1}) = 79.9	
62	4.58×10^{-5}	A	12.89784			ΔH_{subl}(kJ mol^{-1}) = 124.001	
70.9	1.79×10^{-4}	B	6477.132			ΔH_{fus}/(kJ mol^{-1}) = 39.9	
71	1.58×10^{-4}	C	273.15			ΔS_{fus}/(J mol^{-1} K^{-1}) = 69	
71.1	1.59×10^{-4}						
		Antoine eq. for 305–420 °C					
eq. 1	P/Pa	eq. 2	P/mmHg				
A	34.570834	A	8.78307				
B	14903.438	B	4098.173				
		C	273.15				

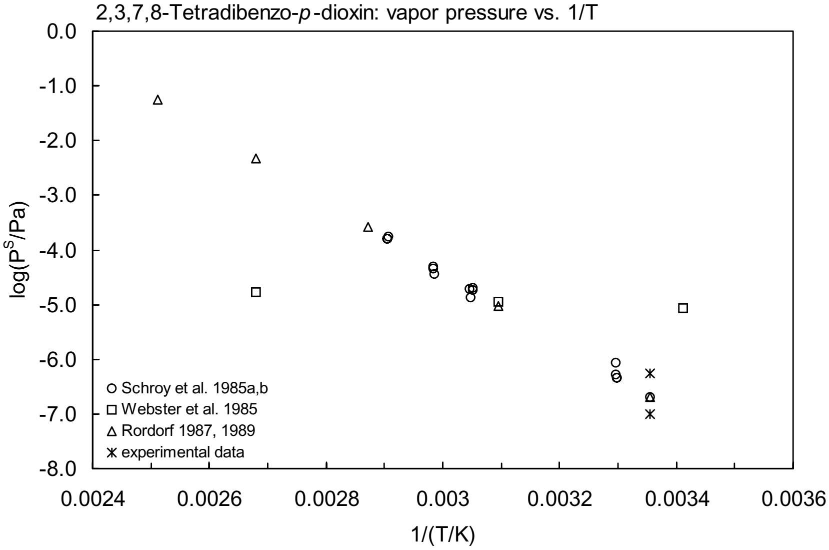


FIGURE 8.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.

TABLE 8.1.1.16.2
Reported octanol-air partition coefficients of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin at various temperatures

	Harner et al. 2000
	generator column-GC/ECD
t/°C	K_{OA}
20	10.318
40	9.283
50	8.778
25	10.05
log K_{OA} = a + b/(T/K)	
a	–6.19
b	4840
enthalpy of phase change	
ΔH_{OA}/(kJ mol^{-1}) = 92.60	

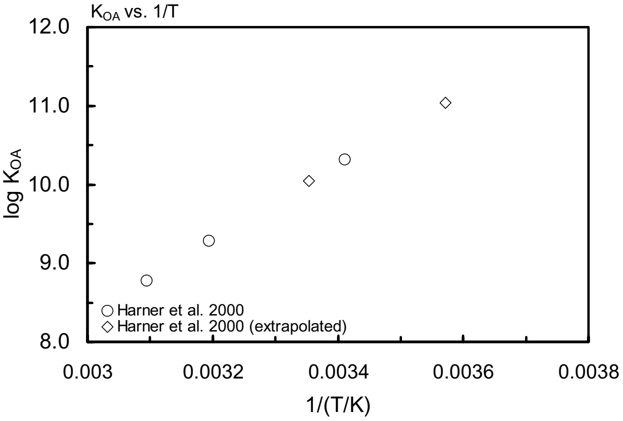
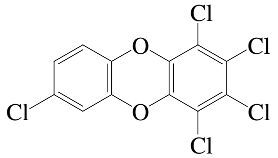


FIGURE 8.1.1.16.2 Logarithm of K_{OA} versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.

8.1.1.17 1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,4,7-P_5CDD
Chemical Name: 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin
CAS Registry No: 39227–61–7
Molecular Formula: $ClC_6H_3O_2C_6Cl_4$
Molecular Weight: 356.416
Melting Point (°C):
195 (Lide 2003)
Boiling Point (°C):
464.7 (calculated, Rordorf 1987, 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
197.74 (calculated-liquid density, Govers et al. 1990)
281.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
92.8 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
137.419 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
42.4 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
26 (Friesen & Webster 1990)
Entropy of Fusion, ΔS_{fus} (J/mol K):
90 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0215 (mp at 195°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
0.000118*; 0.0000855 (20°C, ^{14}C-labelled, generator column-HPLC/LSC, measured range 20–40°C, calculated, Friesen et al. 1985)
0.0000955 (20°C, ^{14}C-labeled, generator column-HPLC/LSC, Webster et al. 1986)
1.23×10^{-4}* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)
0.00428 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
8.80×10^{-8}* (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987,1989)
1.00×10^{-6} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
1.00×10^{-6} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
$\log (P/Pa) = 17.02207 - 7179.05/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
4.57×10^{-6} (supercooled liquid P_L, GC-RI correlation; Wang & Wong 2002)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.264 (calculated-P/C, Shiu et al. 1988; quoted, Kaupp & McLachlan 1999)
0.224; 1.23 (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
0.691; 1.23 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

9.44, 9.62, 10.02; 9.39, 9.65, 10.05 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
9.40, 9.65 (HPLC-RT correlation, Sarna et al. 1984)
9.48, 8.80; 9.40, 8.64 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
9.65, 7.44 (HPLC-RT correlation, Burkhard & Kuehl 1986)
6.60 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)
7.53 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

10.67*; 10.32 (generator column-GC; calculated, Harner et al. 2000)
log K_{OA} = –7.65 + 5460/(T/K), temp range 30–50°C (Harner et al. 2000)
10.42 (GC-retention time correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.26 (fathead minnow, steady-state, wet weight, Muir et al. 1985)
2.50 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
3.16, 2.91 (fathead minnow, rainbow trout, De Voogt et al. 1990;)
3.50, 4.50 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
5.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

4.85, 4.60, 4.50 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986b)
5.80, 5.67, 5.90 (20, 30, 40°C, humic acid from Manitoba peat bog, Webster et al. 1986b)
6.38, 6.39, 6.46 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986b)
5.02 (DOC, De Voogt et al. 1990)
8.57 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant k = 4.31×10^{-6} s^{-1} in water-acetonitrile (2:3, v/v) at 313 nm and calculated half-lives under conditions of variable sunlight intensity at 40°N latitude: $t_{1/2}$ = 18.29 d in spring with rate constant k = 0.466×10^{-6} s^{-1}, $t_{1/2}$ = 15.16 d in summer with k = 0.562×10^{-6} s^{-1}, $t_{1/2}$ = 28.59 d in fall with k = 0.298×10^{-6} s^{-1}, $t_{1/2}$ = 52.37 d in winter with k = 0.163×10^{-6} s^{-1}, and $t_{1/2}$ = 76.82 d averaged over full year with rate constant k = 0.111×10^{-6} s^{-1} (Choudhary & Webster 1985a, 1986);

k = 4.3115×10^{-6} s^{-1} in water-acetonitrile (3:3 v/v) at 313 nm (Choudhary & Webster 1985b);

photolysis k = 4.31×10^{-6} s^{-1} with $t_{1/2}$ = 45.86 h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: k = 4.03×10^{2} d^{-1} with $t_{1/2}$ = 18 d in spring, k = 4.86×10^{2} d^{-1} with $t_{1/2}$ = 15 d in summer, k = 2.58×10^{2} d^{-1} with $t_{1/2}$ = 29 d in fall, k = 1.41×10^{2} d^{-1} with $t_{1/2}$ = 52 d in winter (Choudhary & Webster 1989);

k = 0.74 d^{-1} under mid-summer sunlight at 50°N latitude in filtered-sterilized natural water and k = 0.058 d^{-1} in (2:3, v/v) distilled water-acetonitrile (Friesen et al. 1990);

photolytic $t_{1/2}$ = 38 h in fly-ash extract (Tysklind & Rappe 1991);

$t_{1/2}$ = 92 h for photodegradation in a rotary photoreactor adsorbed to clean silica gel by filtered <290 nm of light (Koester & Hites 1992).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (12 – 14) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (6.5 – 14) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 1.1–2.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^{6} molecule cm^{-3} at room temp. (Atkinson 1991)

k_{OH}(calc) = (1.7 – 3.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 4.0–8.5 d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation: biotransformation rate constant k = 0.014 d^{-1} for rainbow trout (Sijm et al. 1990).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 285 d^{-1}; k_2 = 0.22 d^{-1} (fathead minnow, flow-through system, Muir et al. 1985)
k_1 = 204 d^{-1}; k_2 = 0.28 d^{-1} (rainbow trout, flow-through system, Muir et al. 1985)
k_2 = 2.5 × 10^{-2}, 3.9 × 10^{-2} d^{-1} (rainbow trout for 2 to 21 d exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1990)
k_1 = 509, 162 L kg^{-1} d^{-1}; k_2 < 0.1, > 1.5 d^{-1} (goldfish after 120-h exposure for metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
k_1 = 169 L kg^{-1} d^{-1}, 251 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:
Air: tropospheric lifetime of 1.1–2.4 d calculated for the gas-phase with OH radicals using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3, (Atkinson 1991);
photodegradation $t_{½}$ = 92 h in a rotary photo-reactor adsorbed to clean silica gel by filtered λ < 290 nm of light (Koester & Hites 1992);
calculated tropospheric lifetime of 4.0–8.5 d for penta-chlorinated dioxin for the gas-phase reaction with OH radical at room temp. (Kwok et al. 1995);
suggested $t_{½}$ = 200 h at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000).
Surface water: under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile solution (4:6, v/v): $t_{½}$ = 18.29 d in spring, $t_{½}$ = 15.16 d in summer, $t_{½}$ = 28.6 d in fall, $t_{½}$ = 52.37 d in winter, and $t_{½}$ = 76.82 d averaged over full year (Choudhary & Webster 1985a,1986);
photolysis $t_{½}$ = 45.86 h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct phototransformation half-lives near water bodies at 40°N latitude: $t_{½}$ = 18.4 d in spring, $t_{½}$ = 15 d in summer, $t_{½}$ = 29 d in fall and $t_{½}$ = 52 d in winter (Choudhary & Webster 1989);
$t_{½}$ = 27 d in sunlit surface water and $t_{½}$ = 0.94 d in surface water of actual pond (Friesen et al. 1990).
Groundwater:
Sediment: degradation half-lives in sediment 20–200 yr for all homologues (estimated, Suzuki et al. 2000).
Soil: degradation half-lives in soil 10–100 yr (estimated, Suzuki et al. 2000).
Biota: $t_{½}$ = 3.1 d in fathead minnow (Adams et al. 1986);
$t_{½}$ = 2 d in whole body of rainbow trout (Muir & Yarechewski 1988);
half-lives in gold fish: $t_{½}$ >7 d for PBO treated and $t_{½}$ <0.5 d for control fish in 120-h exposure studies (Sijm et al. 1993).

TABLE 8.1.1.17.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OA}
20	1.20 × 10^{-4}	7	5.05 × 10^{-5}	25	8.8 × 10^{-8}	20	10.996
40	3.17 × 10^{-4}	11.5	6.70 × 10^{-5}	50	6.4 × 10^{-6}	40	9.751
		17	8.70 × 10^{-5}	75	2.5 × 10^{-4}	50	9.282
		21	1.24 × 10^{-4}	100	6.1 × 10^{-3}	25	10.67
		26	1.65 × 10^{-4}	125	9.8 × 10^{-2}		
		41	4.56 × 10^{-4}			log K_{OA} = a + b/(T/K)	

(*Continued*)

TABLE 8.1.1.17.1 (*Continued*)

Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OA}
				ΔH_V/(kJ mol^{-1}) = 92.8		a	–7.65
		ΔH_{sol}/(kJ mol^{-1}) = 47.5		ΔH_{subl}/(kJ mol^{-1}) = 131.42		b	5460
		7–41 °C		ΔH_{fus}/(kJ mol^{-1}) = 42.4		enthalpy of phase change	
				ΔS_{fus}/(J mol^{-1} K^{-1}) = 90		ΔH_{OA}/(kJ mol^{-1}) = 104.0	

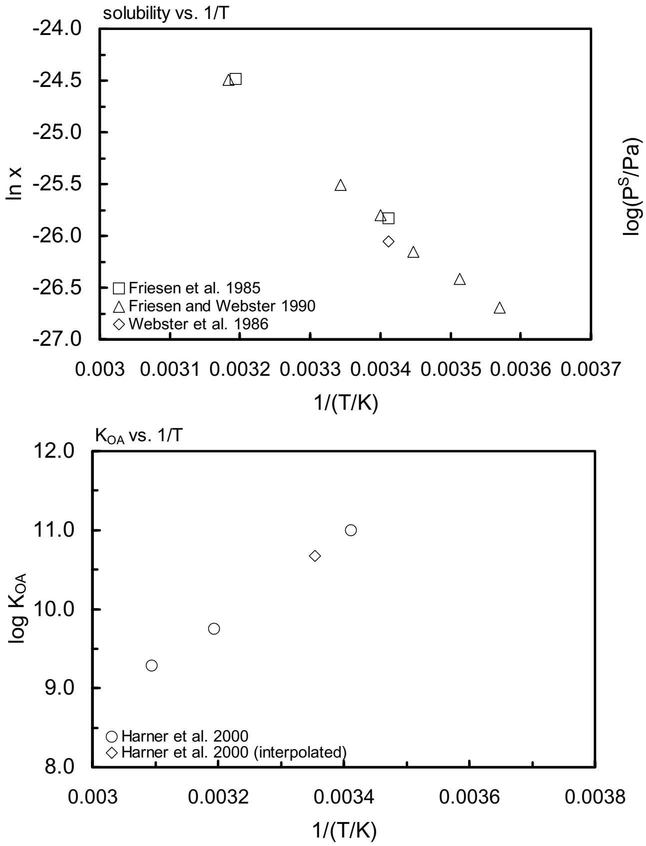
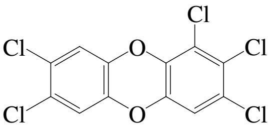


FIGURE 8.1.1.17.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin.

8.1.1.18 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,7,8-P_5CDD
Chemical Name: 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin
CAS Registry No: 40321–76–4
Molecular Formula: $Cl_2C_6H_2O_2C_6HCl_3$
Molecular Weight: 356.416
Melting Point (°C):
Boiling Point (°C):
464.7 (calculated, Rordorf 1987, 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
195.74 (calculated-liquid density, Govers et al. 1990)
281.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
88.7 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
134.062 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
42.4 (Rordorf 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
83 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.000722 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and the reported temperature dependence equations):
9.82×10^{-5} (calculated-QSAR, Fielder & Schramm 1990)
2.77×10^{-3} (supercooled liquid S_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(\text{mol/L})] = 0.445 - 2232/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
4.0×10^{-3}; 2.77×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
5.80×10^{-8}* (calculated, Rordorf 1985a,b, 1987,1989; quoted, Kaupp & McLachlan 1999)
1.20×10^{-5} (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
1.71×10^{-4}; 1.23×10^{-7} (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/\text{Pa}) = 12.72 - 5850/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 8.38 - 3321/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
4.17×10^{-6}; 1.20×10^{-5} (supercooled liquid P_L; GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m^3/mol at 25°C and the reported temperature dependence equations):
1.48 (calculated-SOFA model, Govers & Krop 1998)
$\log (H/(\text{Pa m}^3/\text{mol})) = 7.94 - 1089/(T/K)$ (Passivirta et al. 1999)
0.661; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.64 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989a)
7.50 (calculated-SOFA model, Govers & Krop 1998)
7.27 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)

7.215 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.55; 7.50 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
6.78, 6.84, 6.49, 6.87 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

10.57*; 10.44 (generator column-GC; calculated, Harner et al. 2000)
11.63 (7°C, GC-retention time correlation, Harner et al. 2000)
log K_{OA} = –8.02 + 5540/(T/K); temp range 30–50°C (generator column-GC/ECD, Harner et al. 2000)
10.46 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.20 (guppy, exposed to fly ash extract, Opperhuizen et al. 1986)
3.93; 4.31 (goldfish: PBO treated; control, 120-h exposure, Sijm et al. 1993)
5.27 (guppies, 21-d exposure, system-I absence of sediment, Loonen et al. 1994b)
4.98 (guppies, 21-d exposure, system-II with sediment, Loonen et al. 1984b)
5.34 (calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

5.91 (calculated-QSAR, Fiedler & Schramm 1990)
6.80 (Baltic sea particulate field samples, concentration distribution-GC/MS, Broman et al. 1991)
8.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: solution photolysis $t_{½}$ = 456 min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{½}$ = 52.8 min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984);

photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with $t_{½}$ = 33.6 h for native congener and $t_{½}$ = 16.7 h for ^{13}C-labeled congener in tetradecane solution (Tysklind & Rappe 1991);

$t_{½}$ = 57.8 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) =6.5 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (6.5 – 14) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 1.1–2.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5 × 10^6 molecule cm^{-3} at room temp. (Atkinson 1991)

k_{OH}(calc) = (1.7 – 3.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 4.0–8.5 d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 700 mL g^{-1} d^{-1}; k_2 = 0.090 d^{-1} (guppy, Opperhuizen et al. 1986)

k_1 = 127, 695 L kg^{-1} d^{-1}; k_2 = 0.02, < 0.1 d^{-1} (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure, Sijm et al. 1993)

k_1 = 169 L kg^{-1} d^{-1}, 251 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_1 = 952 L kg^{-1} d^{-1}; k_2 = 0.030 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

k_2 = 0.0051 d^{-1} with $t_{½}$ = 50 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: for a penta-chlorinated dioxin, using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3, the tropospheric lifetime τ = 1.1–2.4 d for the gas phase with OH radical (Atkinson 1991);

calculated tropospheric lifetime τ = 4.0–8.5 d for reaction with OH radical (Kwok et al. 1995);
$t_{½}$ = 360 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: $t_{½}$ = 7200 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Groundwater:
Sediment: $t_{½}$ = 1000000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
degradation $t_{½}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000).
Soil: $t_{½}$ = 1,000,000 h at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000);
degradation $t_{½}$ = 10–100 yr in soil (estimated, Suzuki et al. 2000).
Biota: half-lives in gold fish: $t_{½}$ = 32 d for PBO treated and $t_{½}$ >7 d for control fish in 120-h exposure studies (Sijm et al. 1993);
$t_{½}$ = 49 d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.18.1
Reported vapor pressures and octanol-air partition coefficients of 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin at various temperatures

Vapor pressure		log K_{OA}	
Rordorf 1987, 1989		Harner et al. 2000	
vapor pressure correlation		generator column-GC/ECD	
t/°C	P/Pa	t/°C	log K_{OA}
25	5.8×10^{-8}	20	10.867
50	3.8×10^{-6}	40	9.755
75	1.4×10^{-4}	50	9.083
100	3.0×10^{-3}	25	10.57
125	4.6×10^{-2}		
		log K_{OA} = a + b/(T/K)	
$\Delta H_V/(kJ\ mol^{-1})$ = 88.7		a	−8.02
$\Delta H_{sub}/(kJ\ mol^{-1})$ = 138.062		b	5540
$\Delta H_{fus}/(kJ\ mol^{-1})$ = 42.4			
		$\Delta H_{OA}/(kJ\ mol^{-1})$ = 106 for GC-RT correlation	

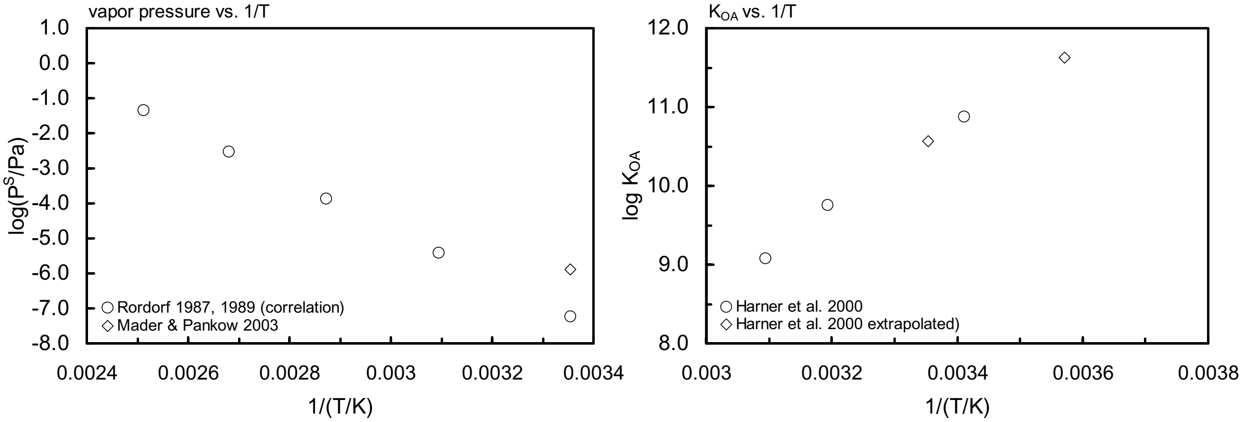
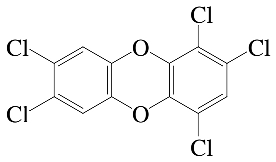


FIGURE 8.1.1.18.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin.

8.1.1.19 1,2,4,7,8-Pentachlorodibenzo-*p*-dioxin



Common Name: 1,2,4,7,8-Pentachlorodibenzo-*p*-dioxin
Synonym: 1,2,4,7,8-P_5CDD
Chemical Name: 1,2,4,7,8-pentachlorodibenzo-*p*-dioxin
CAS Registry No: 58802–08–7
Molecular Formula: $Cl_2C_6H_2O_2C_6HCl_3$
Molecular Weight: 356.416
Melting Point (°C):
 206 (Rordorf 1987)
Boiling Point (°C):
 464.7 (calculated, Rordorf 1987, 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
 199.91 (calculated-liquid density, Govers et al. 1990)
 281.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 91.8 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
 136.636 (Rordorf 1987)
 125.3 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 42.4 (Rordorf 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 88 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0168 (mp at 206°C)

Water Solubility (g/m^3 or mg/L at 25°C):
 9.82×10^{-5} (calculated-QSAR, Fielder & Schramm 1990)
 4.92×10^{-3} (supercooled liquid S_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 5.39×10^{-3}; 4.92×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):
 7.80×10^{-8}, 5.6×10^{-6}, 2.1×10^{-4}, 5.1×10^{-3}, 8.0×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
 1.58×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
 6.026×10^{-6}; 1.58×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
 $\ln (P/Pa) = 38.743 - 16431/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
 $\ln (P/Pa) = (36.472 \pm 0.679) - (15073 \pm 282)/(T/K)$; temp range 403–428 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol):
 1.096 (calculated-SOFA model, Govers & Krop 1998)
 7.41; 1.096 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
 6.64 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)
 8.41 (calculated-QSAR, Fiedler & Schramm 1990)
 7.36 (calculated-SOFA model, Govers & Krop 1998)

7.46; 7.36 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
6.20; 6.71, 6.78, 6.55, 6.87 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

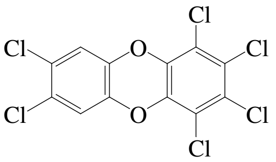
Bioconcentration Factor, log BCF:
5.34 (calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:
5.91 (calculated-QSAR, Fiedler & Schramm 1990)
8.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Volatilization:
Photolysis: $t_{½}$ = 81.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 6.5×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)
k_{OH} = $(6.5 - 14) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime of 1.1 – 2.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^6 molecule cm^{-3} at room temp. (Atkinson 1991)
k_{OH}(calc) = $(1.7 - 3.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 4.0–8.5 d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 61, 164 L kg^{-1} d^{-1}; k_2 = 0.21, > 1.9 d^{-1} (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure, Sijm et al. 1993)
k_1 = 169 L kg^{-1} d^{-1}, 251 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:
Air: tropospheric lifetime τ = 1.1–2.4 d calculated for a penta-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime τ = 2.8–7.2 d for the gas-phase reaction with OH radical (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment: degradation $t_{½}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000).
Soil: degradation $t_{½}$ = 10–100 yr in soil (estimated, Suzuki et al. 2000).
Biota: half-lives in gold fish: $t_{½}$ = 3.3 d for PBO treated and $t_{½}$ >1.9 d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.20 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,4,7,8-H_6CDD
Chemical Name: 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin
CAS Registry No: 39227–26–8
Molecular Formula: $Cl_2C_6H_2O_2C_6Cl_4$
Molecular Weight: 390.861
Melting Point (°C):
  273–275 (Pohland & Yang 1972; Rordorf 1987,1989; Delle Site 1997)
Boiling Point (°C):
  487.7 (calculated, Rordorf 1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  206.96 (calculated-liquid density, Govers et al. 1990)
  302.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  89.1 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
  140.782 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  48.1 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
  30.21 (Friesen & Webster 1990)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  88 (Rordorf 1987, 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F: 0.00369 (assuming ΔS_{fus} = 56 J/mol K and mp at 273°C)
  0.00352 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)
  0.000148 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  4.40×10^{-6}* (20°C, ^{14}C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)
  5.70×10^{-6} (20°C, ^{14}C-labeled, generator column-HPLC/LSC, Webster et al. 1986b)
  4.89×10^{-6}* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)
  log [S_L/(mol/L)] = 0.235 B 2515/(T/K) (supercooled liquid, Passivirta et al. 1999)
  1.15×10^{-3} (supercooled liquid S_L; GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
  5.10×10^{-9}* (calculated-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
  3.20×10^{-7} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
  3.96×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)
  5.43×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
  1.00×10^{-8} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
  1.45×10^{-6} (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
  1.36×10^{-9}, 1.87×10^{-9} (solid P_S, calculated from reported P_L, Delle Site 1997)
  3.19×10^{-6} (corrected supercooled liquid P_L, Eitzer & Hites 1998)
  5.20×10^{-5}; 7.70×10^{-9} (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

log (P_S/Pa) = 12.97 – 6282/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 8.37 – 3769/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P/Pa) = 15.65106 – 7087.08/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
3.72×10^{-5} (supercooled liquid P_L, Harner et al. 2000)
8.91×10^{-7} (supercooled liquid P_L; GC-RI correlation; Wang & Wong 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
0.452 (calculated-P/C, Shiu et al. 1988; quoted, Kaupp & McLachlan 1999)
0.631; 1.45 (quoted lit., calculated-SOFA model, Govers & Krop 1998)
log (H/(Pa m^3/mol)) = 8.14 – 1254/(T/K) (Passivirta et al. 1999)
0.427; 1.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
10.36, 10.39, 10.89; 10.22, 10.44, 10.89 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
10.40, 9.65; 10.22, 9.19 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
10.44, 7.79 (HPLC-RT correlation, Burkhard & Kuehl 1986)
7.80 (selected, Shiu et al. 1988)
8.0 (calculated-QSAR, Fiedler & Schramm 1990)
7.30 (calculated, Broman et al. 1991)
9.53 (HPLC-RT correlation, Chessells et al. 1991)
9.13 (calculated-fragment const., Chessells et al. 1991)
10.22 (quoted, Hansch et al. 1995)
7.94 (calculated-SOFA model, Govers & Krop 1998)
7.90 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
7.628 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.94; 7.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
7.80; 7.12, 7.12, 7.25, 7.30 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
11.50 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
11.17 (calculated, Finizio et al. 1997)
11.11*; 10.88 (generator column-GC; calculated, Harner et al. 2000)
12.20 (7°C, GC-retention time correlation, Harner et al. 2000)
log K_{OA} = –6.20 + 5160/(T/K); temp range 30–50°C (generator column-GC/ECD, Harner et al. 2000)
10.95 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:
3.73, 4.00 (rainbow trout, fathead minnow, steady-state, wet weight, Muir et al. 1985)
4.00, 5.00 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
3.41, 3.76 (fathead minnow, quoted, Opperhuizen & Sijm 1990)
3.45, 3.23 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
3.45, 4.87 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
5.01; 4.65 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
5.01; 5.01; 5.14 (guppy, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
5.01; 5.07 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
5.90, 5.98 (fish muscle log BCF_L calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
5.41, 5.31, 5.13 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986)
6.02, 6.15, 5.95 (20, 30, 40°C, humic acid from Manitoba peat bog, Webster et al. 1986)
6.32, 6.27, 6.15 (20. 30. 40°C, Aldrich humic acid, Na salt, Webster et al. 1986b)
5.02 (DOC, De Voogt et al. 1990)
7.10 (Baltic Sea particulate field samples, concentration distribution-GC/MS, Broman et al. 1991)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

k(calc) = 1.06×10^{-6} s^{-1} with $t_{½}$ = 7.57 d in spring, k = 1.280×10^{-6} s^{-1} with $t_{½}$ = 6.27 d in summer, k = 0.676×10^{-6} s^{-1} with $t_{½}$ = 11.87 d in autumn, k = 0.37×10^{-6} s^{-1} with $t_{½}$ = 21.57 d in winter and the averaged k = 0.252×10^{-6} s^{-1} over full year with $t_{½}$ = 31.85 d, under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile (4:6 v/v) solution (Choudhary & Webster 1985a,c, 1986)

k = 7.86×10^{-6} s^{-1} in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhary & Webster 1985b)

k = 7.86×10^{-6} s^{-1} with $t_{½}$ = 24.5 h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: k = 9.16×10^{2} d^{-1} with $t_{½}$ = 7.6 d in spring, k = 11.06×10^{2} d^{-1} with $t_{½}$ = 6.3 d in summer, k = 5.84×10^{2} d^{-1} with $t_{½}$ = 12.0 d in fall, k = 3.21×10^{2} d^{-1} with $t_{½}$ = 22.0 d in winter (Choudhary & Webster 1989)

k = 0.28 d^{-1} in natural water and k = 0.019 d^{-1} in distilled water-acetonitrile (Friesen et al. 1990)

photolytic $t_{½}$(calc) = 38 h in the fly ash extract in tetradecane (Tysklind & Rappe 1991)

photodegradation $t_{½}$ = 140 h in a rotary photoreactor absorbed to silica gel by filtered < 290 nm of light (Koester & Hites 1992)

$t_{½}$ = 91.8 h on spruce needles surface under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved PCDD is 5.02×10^{4} L g^{-1} min^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = $(4.6 - 5.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(4.6 - 10) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 1.5–3.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^{6} molecule/cm^3 for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 102 d^{-1}; k_2 = 0.046 d^{-1} (rainbow trout, flow-through system, Muir et al. 1985)

k_1 = 112 d^{-1}; k_2 = 0.030 d^{-1} (fathead minnow, Muir et al. 1985)

k_2 = 0.030 d^{-1} (fathead minnow, Muir et al. 1985)

k_2 = 0.015 d^{-1} (rainbow trout, Muir & Yarechewski 1988)

k_2 = 0.0066 d^{-1} (fathead minnow, Muir & Yarechewski 1988)

k_1 = 58 L kg^{-1} d^{-1}, 299 L kg^{-1} d^{-1} (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 = 0.29, > 0.02 d^{-1} (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1993)

k_1= 868 L kg^{-1} d^{-1}; k_2 = 0.065 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

k_2 = 0.0105 d^{-1} with $t_{½}$ = 29 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: estimated reaction rate constant, k = 0.005 h^{-1} (Paterson et al. 1990);

tropospheric lifetime τ = 1.5–3.4 d for a hexa-chlorinated dioxin reaction with the OH radicals using a 12-h average daytime OH radical concn of 1.5×10^{6} molecule/cm^3,(Atkinson 1991);

photodegradation $t_{½}$ = 140 h in a rotary photoreactor adsorbed to clean silica gel by filtered λ < 290 nm of light, (Koester & Hites 1992);

suggested $t_{½}$ = 740 h at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000).

Surface water: under conditions of variable sunlight intensity at 40°N latitude: $t_{½}$ = 7.57 d in spring, $t_{½}$ = 6.27 d in summer, $t_{½}$ = 11.87 d in fall, $t_{½}$ = 21.57 d in winter, and $t_{½}$ = 76.8 d averaged over full year (Choudhary & Webster 1985a, 1986);

photolysis $t_{½}$ = 24.5 h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct phototransformation half-lives near water bodies at 40°N latitude: 7.6 d in spring, 6.3 d in summer, 12.0 d in fall and 22.0 d in winter (Choudhary & Webster 1989);

$t_{½}$ = 81 d in sunlit surface water and $t_{½}$ = 2.5 d in surface water of actual pond (Friesen et al. 1990);

estimated reaction rate constant, k = 0.002 h^{-1} (Paterson et al. 1990);
suggested $t_{1/2}$ = 14800 h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: estimated reaction rate constant k = 4.0×10^{-6} h^{-1} (Paterson et al. 1990);
degradation $t_{1/2}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);
suggested $t_{1/2}$ = 2400000 h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: estimated reaction rate constant k = 2.8×10^{-6} h^{-1} (Paterson et al. 1990);
degradation $t_{1/2}$ =10–100 yr in soil for all homologues (estimated, Suzuki et al. 2000);
$t_{1/2}$ = 2400000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{1/2}$ = 43 d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);
half-lives in gold fish: $t_{1/2}$ = 2.4 d for PBO treated and $t_{1/2}$ = 40 d for control fish in 120-h exposure studies (Sijm et al. 1993);
$t_{1/2}$ = 29 d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.20.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OA}
20	4.40×10^{-6}	7	2.31×10^{-6}	25	5.1×10^{-9}	20	11.403
40	1.90×10^{-5}	11.5	3.12×10^{-6}	50	4.1×10^{-7}	40	10.297
		17	4.18×10^{-6}	75	1.8×10^{-5}	50	9.762
		21	4.89×10^{-6}	100	4.6×10^{-4}	25	11.11
		26	7.90×10^{-6}	125	8.0×10^{-3}		
		41	1.90×10^{-5}			log K_{OA} = a + b/(T/K)	
				ΔH_V/(kJ mol^{-1}) = 89.1		a	–6.20
		ΔH_{sol}/(kJ mol^{-1}) = 45.5		ΔH_{subl}/(kJ mol^{-1}) = 140.78		b	5160
		7–41 °C		ΔH_{fus}/(kJ mol^{-1}) = 48.1		enthalpy of phase change	
				ΔS_{fus}/(J mol^{-1} K^{-1}) = 88		ΔH_{OA}/(kJ mol^{-1}) = 98.70	

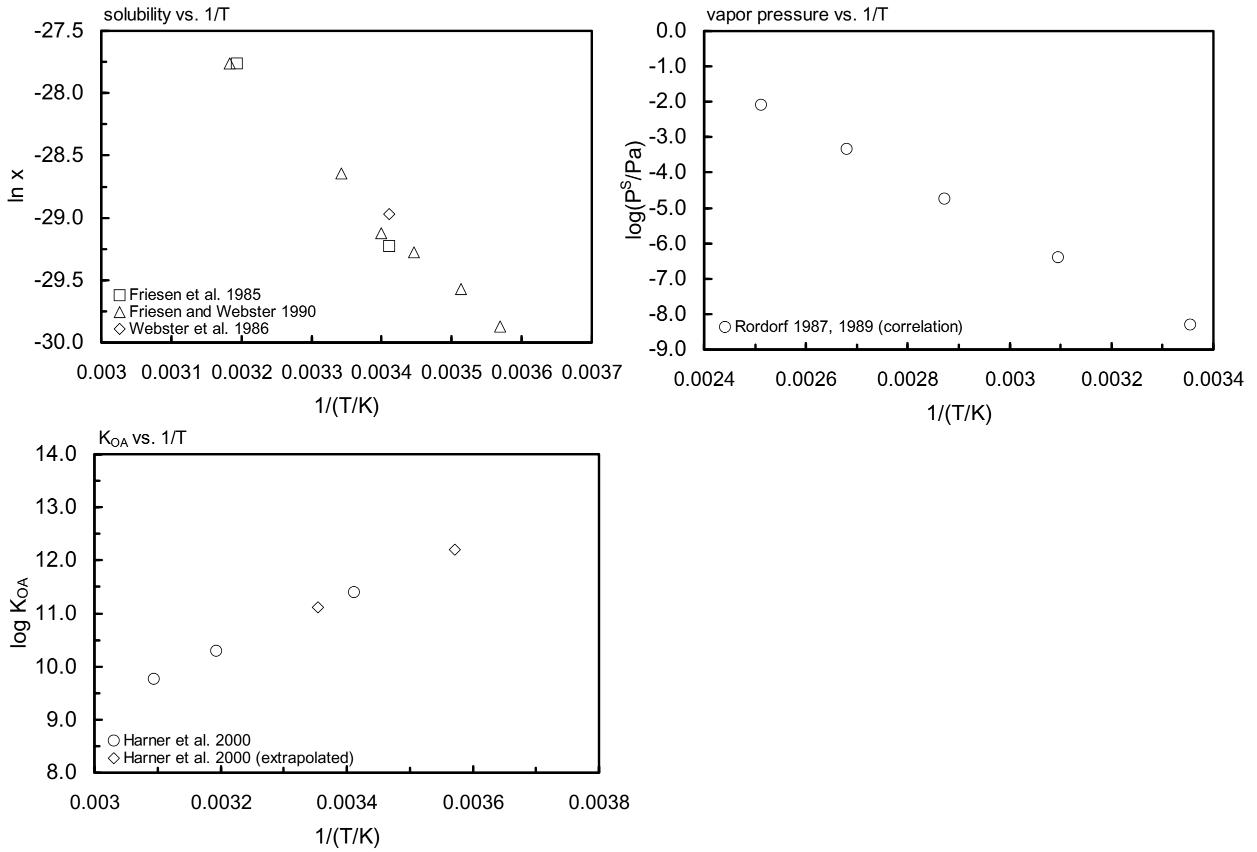
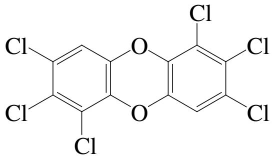


FIGURE 8.1.1.20.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin.

8.1.1.21 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,6,7,8-H_6CDD
Chemical Name: 1,2,3,6,7,8-hexachlorodibenzo-*p*-dioxin
CAS Registry No: 57653–85–7
Molecular Formula: $Cl_3C_6HO_2C_6HCl_3$
Molecular Weight: 390.861
Melting Point (°C):
285 (Lide 2003)
Boiling Point (°C):
487.7 (calculated, Rordorf 1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
207.16 (calculated-liquid density, Govers et al. 1990)
302.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
88.1 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
139.975 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
48.1 (Rordorf 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
86 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C, F: 0.00281 (assuming ΔS_{fus} = 56 J/mol K and mp at 185°C)
0.000167 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and the reported temperature dependence equations):
8.75×10^{-4} (calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(\text{mol/L})] = 0.125 - 2515/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
1.10×10^{-3}, 8.75×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):
4.80×10^{-9}, 3.80×10^{-7}, 1.60×10^{-5}, 4.0×10^{-4}, 6.9×10^{-3} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
3.31×10^{-6} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
5.20×10^{-5}; 8.69×10^{-9} (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/\text{Pa}) = 12.96 - 6363/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 8.47 - 3751/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
8.51×10^{-7}, 3.31×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m^3/mol at 25°C and the reported temperature dependence equations):
1.45 (calculated-SOFA model, Govers & Krop 1998)
$\log [H/(\text{Pa m}^3/\text{mol})] = 8.35 - 1236/(T/K)$ (Passivirta et al. 1999)
0.417; 1.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
9.13 (calculated-QSAR, Fiedler & Schramm 1990)
7.80 (calculated, Broman et al. 1991)

7.98 (calculated-SOFA model, Govers & Krop 1998)
7.96 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
7.639 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.94; 7.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
7.58 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.22 (7°C, GC-retention time correlation, Harner et al. 2000)
10.97 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:
3.41, 4.61 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
4.94; 4.70 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.94; 5.05; 5.24 (guppies, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
5.98 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
5.56 (fish muscle log BCF_L calculated from water, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
7.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
9.42 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: solution photolysis $t_{½}$ = 379 min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{½}$ = 44100 min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984);

photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with $t_{½}$ = 17.3 h for native congener and $t_{½}$ = 14.2 h for ^{13}C-labeled congener in tetradecane solution (Tysklind & Rappe 1991);

$t_{½}$ = 76.2 h on spruce needle surface under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(4.6 - 5.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(4.6 - 10) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and a calculated tropospheric lifetime τ = 1.5–3.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^6 molecule/cm^3 for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 432 L kg^{-1} d^{-1} (goldfish after 120-h exposure, control fish, Sijm et al. 1993)

k_1 = 58 L kg^{-1} d^{-1}, 299 L kg^{-1} d^{-1} (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 = 0.23, < 0.1 d^{-1} (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_1 = 844 L kg^{-1} d^{-1}; k_2 = 0.050 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

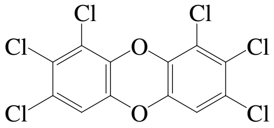
k_2 = 0.0075 d^{-1} with $t_{½}$ = 60 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991);

$t_{½}$ = 740 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: $t_{½}$ = 14800 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: degradation $t_{½}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);
$t_{½}$ = 550000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
Soil: degradation $t_{½}$ = 10–100 yr in soil for all homologues (estimated, Suzuki et al. 2000);
$t_{½}$ = 550 000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
Biota: 43 d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);
$t_{½}$ = 3.0 d for PBO treated gold fish, $t_{½}$ >7 d for control fish in 120-h exposure studies (Sijm et al. 1993);
$t_{½}$ = 40 d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

8.1.1.22 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,7,8,9-H_6CDD OR 2,3,4,6,7,8-H_6CDD
Chemical Name: 1,2,3,7,8,9-hexachlorodibenzo-*p*-dioxin
CAS Registry No: 19408–74–3
Molecular Formula: $Cl_3C_6HO_2C_6HCl_3$
Molecular Weight: 390.861
Melting Point (°C):
243–244 (Rordorf 1987)
Boiling Point (°C):
487.7 (calculated, Rordorf 1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
207.16 (calculated-liquid density, Govers et al. 1990)
210.16 (liquid molar volume, Govers et al. 1995)
301.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
91.7 (Rordorf 1987)
103.9 (GC-RI correlation, Govers et al. 1995)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
142.922 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
48.1 (Rordorf 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
93 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C, F:
0.00027 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and the reported temperature dependence equations):
6.34×10^{-4} (calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(mol/L)] = 0.491 - 2515/(T/K)$ (liquid, Passivirta et al. 1999)
1.10×10^{-3}, 6.34×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
6.50×10^{-9}, 5.60×10^{-7}, 2.60×10^{-5}, 7.00×10^{-4}, 1.30×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
1.38×10^{-6} (calculated-SOFA model, Govers & Krop 1998)
4.51×10^{-5}; 1.22×10^{-8} (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 12.93 - 6211/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 8.07 - 3699/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
8.51×10^{-7}, 1.38×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m^3/mol at 25°C and the reported temperature dependence equations):
0.832 (calculated-SOFA model, Govers & Krop 1998)
$\log [H/(Pa\ m^3/mol)] = 7.58 - 1184/(T/K)$ (Passivirta et al. 1999)
0.417; 0.832 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.90 (calculated, Broman et al. 1991)

8.02 (calculated-SOFA model, Govers & Krop 1998)
7.76 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
7.61 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.95; 8.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
7.58 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.26 (7°C, GC-retention time correlation, Harner et al. 2000)
11.01 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:
2.95 (guppy exposed to fly ash extract, Opperhuizen et al. 1986)
3.50, 4.02 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
4.93; 4.34 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.99; 4.94; 5.02 (guppies, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from nonlinear regression analysis, Loonen et al. 1994b)
5.18 (calculated-SOFA model, Govers & Krop 1998)
5.29 (fish muscle log BCF_L calculated from water, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
6.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
9.45 (calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis: photolytic $t_{½}$ = 5.4 h when exposed to sunlight in hexane solution (Doobs & Grant 1979)
photolytic degradation $t_{½}$ = 17.1 h in extract from fly ash exposed to UV light from a distance of 20 cm in tetradecane solution (Tysklind & Rappe 1991)
$t_{½}$ = 92.4 h on spruce needle surface under sunlight irradiation (Niu et al. 2003).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k (oxidative degradation rate constant of water dissolved PCDD) is 5.02×10^4 L g^{-1} min^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)
k_{OH}(calc) = $(4.6 - 5.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)
k_{OH} = $(4.6 - 10) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime of 1.5 – 3.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^6 molecule cm^{-3} for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 200 mL g^{-1} d^{-1}; k_2 = 0.210 d^{-1} (guppy, Opperhuizen et al. 1986)
k_1 = 48, 433 L kg^{-1} d^{-1}; k_2 = 0.44, < 0.1 d^{-1} (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)
k_1 = 58 L kg^{-1} d^{-1}, 299 L kg^{-1} d^{-1} (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
k_1 = 687 L kg^{-1} d^{-1}; k_2 = 0.074 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)
k_2 = 0.0057 d^{-1} with $t_{½}$ = 52 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3}, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991)

$t_{½}$ = 740 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_{½}$ = 14800 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{½}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);

$t_{½}$ = 2400000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

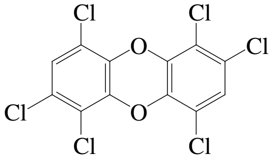
Soil: degradation $t_{½}$ = 10–100 yr in soil for all homologues (estimated, Suzuki et al. 2000);

$t_{½}$ = 2400 000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: half-lives in gold fish: 1.6 d for PBO treated and $t_{½}$ >7 d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{½}$ = 52 d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

8.1.1.23 1,2,4,6,7,9-Hexachlorodibenzo-*p*-dioxin



Common Name: 1,2,4,6,7,9-Hexachlorodibenzo-*p*-dioxin
Synonym: 1,2,4,6,7,9-H_6CDD
Chemical Name: 1,2,4,6,7,9-hexachlorodibenzo-*p*-dioxin
CAS Registry No: 39227–62–8
Molecular Formula: $Cl_3C_6HO_2C_6HCl_3$
Molecular Weight: 390.861
Melting Point (°C):
238–240 (Pohland & Yang 1972, Rordorf 1987)
Boiling Point (°C):
487.7 (calculated, Rordorf 1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
215.5 (calculated-liquid density, Govers et al. 1990)
302.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
92.1 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
143.238 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
48.1 (Rordorf 1987)
Entropy of Fusion, ΔS_{fus} (J/mol K):
94 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C, F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00187 (calculated-SOFA model, Govers & Krop 1998)
1.71×10^{-3}, 1.87×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
6.80×10^{-9}, 5.9×10^{-7}, 2.7×10^{-5}, 7.5×10^{-4}, 1.40×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
1.41×10^{-6} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
1.35×10^{-6}, 1.41×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.0282 (calculated-SOFA model, Govers & Krop 1998)
0.479; 0.0282 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
7.85 (shake flask/slow stirring-GC/MS, mixture of fly-ash extract, Sijm et al. 1989a)
7.73 (calculated-SOFA model, Govers & Krop 1998)
7.84; 7.73 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
6.85; 7.05, 7.26, 6.96, 7.30 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

5.36 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

8.99 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolytic $t_{½}$ = 47 h when exposed to sunlight in hexane solution (Doobs & Grant 1979); solution photolysis $t_{½}$ = 764 min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{½}$ = 7870 min on a clean glass surface under the same conditions (Nestrick et al. 1980)

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (4.6 – 5.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (4.6 – 10) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 1.5–3.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5 × 10^6 $molecule/cm^3$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 88, 82 L kg^{-1} d^{-1}; k_2 = 0.62, > 0.8 d^{-1} (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 58 L kg^{-1} d^{-1}, 299 L kg^{-1} d^{-1} (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10^6 $molecule/cm^3$, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991)

Surface water:

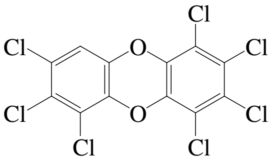
Groundwater:

Sediment: degradation $t_{½}$ = 20–100 yr in sediment for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{½}$ = 10–100 yr in soil or all homologues (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{½}$ = 1.1 d for PBO treated and $t_{½}$ < 0.9 d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.24 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,4,6,7,8-H_7CDD
Chemical Name: 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin
CAS Registry No: 35822–46–9
Molecular Formula: $Cl_3C_6HO_2C_6Cl_4$
Molecular Weight: 425.308
Melting Point (°C):
 264–265 (Rordorf 1987,1989; Delle Site 1997)
Boiling Point (°C):
 507.2 (Rordorf 1987,1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
 218.32 (calculated-liquid density, Govers et al. 1990)
 323.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 92.5 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
 149.792 (Rordorf 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 53.9 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
 30.42 (Friesen & Webster 1990)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 100 (Rordorf 1987,1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F: 0.00442 (assuming ΔS_{fus} = 56 J/mol K and mp at 265°C)
 0.00423 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)
 6.11×10^{-5} (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 2.40×10^{-6}*, 2.42×10^{-6} (20°C, ^{14}C-labeled, generator column-HPLC/LSC, measured range 20–40°C, calculated, Friesen et al. 1985)
 2.30×10^{-6}* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)
 $\log [S_L/(mol/L)] = 0.391 - 2820/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 3.15×10^{-4} (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 7.5×10^{-10}* (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987,1989)
 3.20×10^{-8} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
 1.02×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)
 1.19×10^{-6} (supercooled liquid, GC/MS, Eitzer & Hites 1989)
 3.20×10^{-9} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
 4.41×10^{-9}, 5.15×10^{-9} (solid P_S, calculated from reported P_L, Delle Site 1997)
 8.97×10^{-6} (corrected supercooled liquid P_L, Eitzer & Hites 1998)
 6.03×10^{-7}; 5.89×10^{-7} (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 8.97×10^{-6}; 6.79×10^{-10} (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

log (P_S/Pa) = 13.18 – 6661/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 7.95 – 3844/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P/Pa) = 17.10357 – 7820.06/(T/K) temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
2.04×10^{-7}, 5.89×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m^3/mol at 25°C and the reported temperature dependence equations):
0.133 (calculated-P/C, Shiu et al. 1988)
4.25 (computed-expert system SPARC, Kollig 1995)
0.832 (calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa m^3/mol)] = 7.56 – 7024/(T/K) (Passivirta et al. 1999)
0.275; 0.832 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
11.29, 11.42, 11.90; 11.03, 11.50, 11.98 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
11.05, 11.50 (HPLC-RT correlation, Sarna et al. 1984)
11.38, 10.55; 11.05, 9.69 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
8.20 (HPLC-RT correlation, Burkhard & Kuehl 1986)
11.03 (Hansch et al. 1995)
8.85 (computed-expert system SPARC, Kollig 1995)
8.40 (calculated-SOFA model, Govers & Krop 1998)
8.31 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
8.051 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
8.27; 8.40 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
7.66, 7.43, 8.18, 7.73 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
11.42*; 10.73 (generator column-GC, measured range 20–50°C, calculated, Harner et al. 2000)
log K_{OA} = –3.51 + 4450/(T/K); temp range 30–50°C (Harner et al. 2000)

Bioconcentration Factor, log BCF:
3.32, 3.74 (fathead minnow, rainbow trout, steady-state, wet weight, Muir et al. 1985)
3.32, 4.32 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
2.92, 4.28 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
4.68 (guppy, Loonen et al. 1994)
4.68; 4.08 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.68; 4.68; 4.76 (guppies, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
4.68; 4.79 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
6.11, 6.34 (fish muscle log BCF_L calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
5.47 (DOC, De Voogt et al. 1990)
7.80 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
10.95; 10.0 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
photolytic $t_{½}$ = 11 h in *n*-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)
solution photolysis $t_{½}$ = 1800 min at 1.0 m from a GE Model sunlamp and surface photolysis $t_{½}$ = 3140 min on clean soft glass surface under the same conditions (Nestrick et al. 1980)

$t_{1/2}$ = 30 h in *n*-hexadecane solution (Mamantov 1984);

first order k = 1.02×10^{-6} s^{-1} in water-acetonitrile (2:3, v/v) at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2}$ = 56.46 d in spring; $t_{1/2}$ = 47.33 d in summer; $t_{1/2}$ = 87.86 d in autumn, $t_{1/2}$ = 155.79 d in winter and averaged $t_{1/2}$ 2993 d over full year(Choudhary & Webster 1985b, 1986)

photolysis k = 1.02×10^{-6} s^{-1} with $t_{1/2}$ = 191 h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: k = 1.24×10^{2} d^{-1} with $t_{1/2}$ = 57 d in spring, k = 1.48×10^{2} d^{-1} $t_{1/2}$ = 47 d in summer, k = 0.80×10^{2} d^{-1} with $t_{1/2}$ = 88 d in autumn, k = 0.45×10^{2} d^{-1} $t_{1/2}$ = 156 d in winter (Choudhary & Webster 1989)

sunlight photolysis k = 0.28 d^{-1} in filtered and sterilized natural water and k = 0.019 d^{-1} in (2:32, v/v) distilled water-acetonitrile solution at 50°N (Friesen et al. 1990)

photolytic $t_{1/2}$ = 53.4 for native congener and $t_{1/2}$ = 32.6 h in ^{13}C-labeled congener in extract from fly ash (Tysklind & Rappe 1991)

tropospheric lifetime was calculated based on the gas-phase reaction rate constant k = (4.6–10) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with the OH radicals to be 1.5–2.4 d (Atkinson 1991)

photodegradation rate constant k = 0.18 h^{-1} with $t_{1/2}$ = 3.9 h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000)

$t_{1/2}$ = 83.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved PCDD by ozone) is 5.46×10^{4} L g^{-1} min^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = 3.5×10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 4.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concn of 1.5×10^{6} molecule/cm^3 for a hepta-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 56 d^{-1}; k_2 = 0.042 d^{-1} (rainbow trout exposed to concn of 11, 55 pg/L, Muir et al. 1985)

k_1 = 19 d^{-1}; k_2 = 0.040 d^{-1} (fathead minnow exposed to concn of 8, 39 pg/L, Muir et al. 1985)

k_2 = 0.048 d^{-1} (fathead minnow, Muir & Yarechewski 1988)

k_2 = 0.0092 d^{-1} (fathead minnow, quoted, Opperhuizen & Sijm 1990)

k_2 = 0.0110 d^{-1} (rainbow trout, quoted, Opperhuizen & Sijm 1990)

k_1 = 32, 150 L kg^{-1} d^{-1}; k_2 = 0.49, > 0.12 d^{-1} (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 23 L kg^{-1} d^{-1}, 167 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_1 = 456 L kg^{-1} d^{-1}; k_2 = 0.081 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

k_2 = 0.0061 d^{-1} with $t_{1/2}$ = 49 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^{6} molecule cm^{-3}, the tropospheric lifetime τ = 4.4 d for a hepta-PCDD for the gas-phase reaction with OH radicals (Atkinson 1991);

suggested $t_{1/2}$ = 1500 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000);

first-order photodegradation k = 0.19 h^{-1} with $t_{1/2}$ = 3.9 h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: $t_{1/2}$ = 11 h in *n*-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982);

direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2}$ = 56.46 d in spring; $t_{1/2}$ = 47.33 d in summer; $t_{1/2}$ = 87.86 d in autumn; $t_{1/2}$ = 155.79 d in winter and averaged $t_{1/2}$ = 2393 d over full year (Choudhary & Webster 1985b, 1986);

photolysis $t_{½}$ = 190.97 h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude: $t_{½}$ = 57 d in spring, $t_{½}$ = 47 d in summer, $t_{½}$ = 88 d in fall and $t_{½}$ = 156 d in winter (Choudhary & Webster 1989);

$t_{½}$ = 81 d in sunlit filtered and sterilized surface water and $t_{½}$ = 2.5 d in surface water of actual pond at 50°N latitude (Friesen et al. 1990);

$t_{½}$ = 53.4 and 32.6 h in native and ^{13}C-labeled congeners, respectively, in extract from fly ash (Tysklind & Rappe 1991);

suggested $t_{½}$ = 30000 h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{½}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);

suggested $t_{½}$ = 900000 h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: degradation $t_{½}$ = 10–100 yr in soil (estimated, Suzuki et al. 2000);

suggested $t_{½}$ = 900000 h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Biota: $t_{½}$ = 17.2 d in fathead minnow (Adams et al. 1986);

$t_{½}$ >336 d in carp (Kuehl et al. 1987);

$t_{½}$ = 39 d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);

$t_{½}$ = 27.2 d in lactating cows (Olling et al. 1991);

half-lives in gold fish: $t_{½}$ = 1.4 d for PBO treated and $t_{½}$ = 5.6 d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{½}$ = 49 d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.24.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				**Vapor pressure**		**log K_{OA}**	
Friesen et al. 1985		**Friesen & Webster 1990**		**Rordorf 1987, 1989**		**Harner et al. 2000**	
generator column-HPLC/LSC		**generator column-HPLC/LSC**		**gas saturation-GC**		**generator column-GC/ECD**	
t/°C	**$S/g \cdot m^{-3}$**	**t/°C**	**$S/g \cdot m^{-3}$**	**t/°C**	**P/Pa**	**t/°C**	**log K_{OA}**
20	2.40×10^{-6}	7	9.35×10^{-7}	25	7.5×10^{-10}	20	11.66
40	6.30×10^{-5}	11	1.14×10^{-6}	50	8.0×10^{-8}	40	10.774
		17	1.29×10^{-6}	75	4.4×10^{-6}	50	10.225
		21	2.30×10^{-6}	100	1.4×10^{-4}	25	11.42
		26	2.56×10^{-6}	125	2.9×10^{-3}		
		41	6.34×10^{-5}			log K_{OA} = a + b/(T/K)	
				$\Delta H_V/(kJ\ mol^{-1})$ = 92.5		a	−3.51
		$\Delta H_{sol}/(kJ\ mol^{-1})$ = 42.4		$\Delta H_{subl}/(kJ\ mol^{-1})$ = 149.79		b	4450
		7–41 °C		$\Delta H_{fus}/(kJ\ mol^{-1})$ = 53.9		enthalpy of phase change	
				$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1})$ = 100		$\Delta H_{OA}/(kJ\ mol^{-1})$ = 85.10	

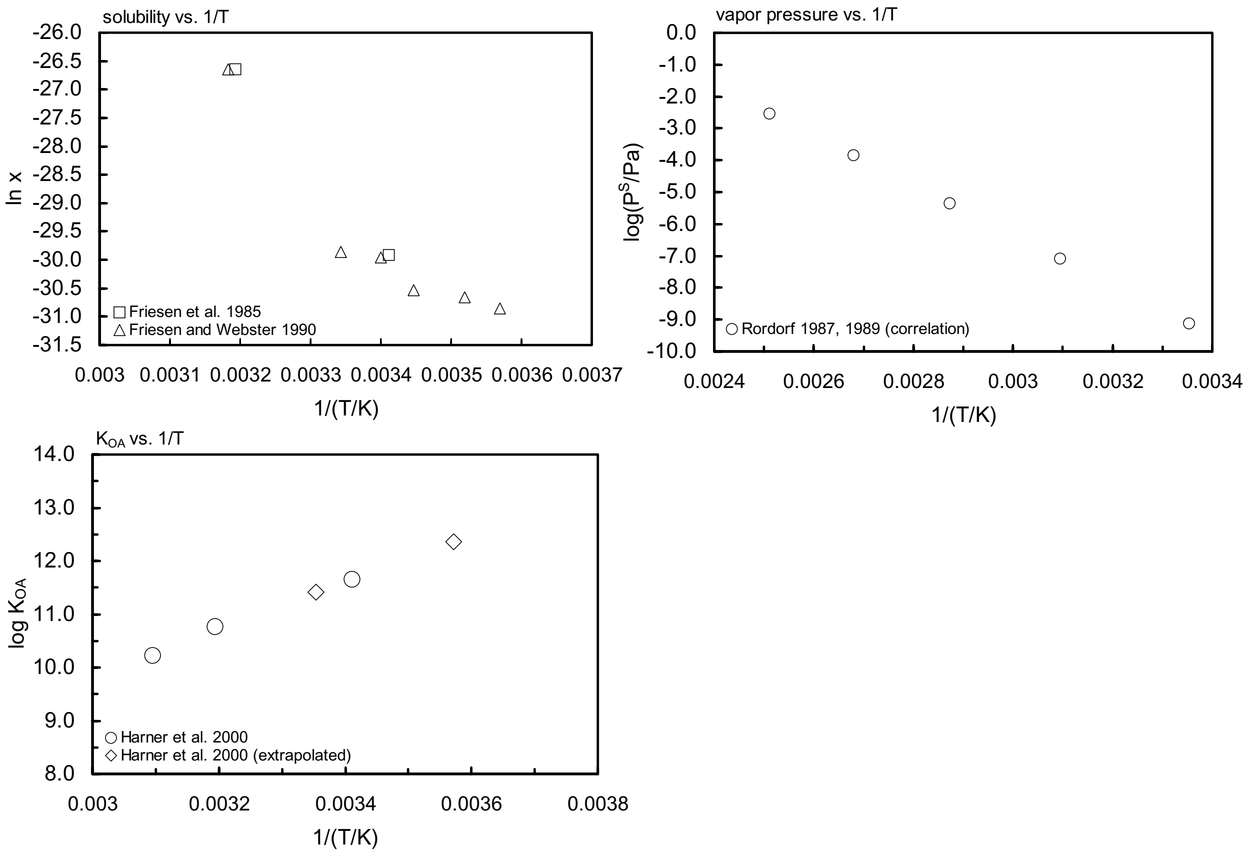
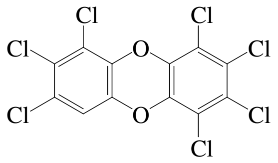


FIGURE 8.1.1.24.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin.

8.1.1.25 1,2,3,4,7,8,9-Heptachlorodibenzo-*p*-dioxin



Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzo-*p*-dioxin
Synonym: 1,2,3,4,7,8,9-H_7CDD
Chemical Name: 1,2,3,4,7,8,9-heptachlorodibenzo-*p*-dioxin
CAS Registry No:
Molecular Formula: $Cl_3C_6HO_2C_6Cl_4$
Molecular Weight: 425.308
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

222.55	(calculated-liquid density, Govers et al. 1990)
323.3	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:

Water Solubility (g/m^3 or mg/L at 25°C):
4.57×10^{-4} (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
3.97×10^{-4}, 4.57×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C):
3.39×10^{-7} (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
2.57×10^{-7}, 3.39×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m^3/mol):

0.309	(calculated-SOFA model, Govers & Krop 1998)
0.295; 0.309	(GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

8.25	(calculated-SOFA model, Govers & Krop 1998)
8.22; 8.25	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

4.95	(lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

9.75	(sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis: photolytic $t_{1/2}$ = 27 h when exposed to sunlight in hexane solution (Dobbs & Grant 1979)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved PCDD by ozone) is 5.46×10^4 L g^{-1} min^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = 3.5×10^{-12} cm^3 $molecule^{-1}$ s^{-1} and a calculated tropospheric lifetime τ = 4.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hepta-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 12 L kg^{-1} d^{-1}, 183 L kg^{-1} d^{-1}; k_2 = 1.3 d^{-1}, >3.4 d^{-1} (metabolic inhibitor PBO-treated goldfish, control goldfish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 22 L kg^{-1} d^{-1}, 167 L kg^{-1} d^{-1} (average k_1 for H_7CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3, the tropospheric lifetime of a hepta-PCDD was calculated to be 4.4 d for the gas-phase reaction with OH radical (Atkinson 1991)

Surface water:

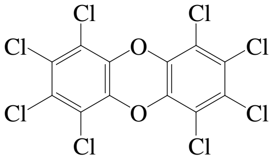
Groundwater:

Sediment: degradation $t_{1/2}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000)

Soil: degradation $t_{1/2}$ = 10–100 yr in soil (estimated, Suzuki et al. 2000)

Biota: half-lives in gold fish: $t_{1/2}$ = 0.5 d for PBO treated and $t_{1/2}$ <0.2 d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.26 Octachlorodibenzo-*p*-dioxin



Common Name: Octachlorodibenzo-*p*-dioxin
Synonym: O_8CDD, OCDD
Chemical Name: octachlorodibenzo-*p*-dioxin
CAS Registry No: 3268–87–9
Molecular Formula: $C_{12}Cl_8O_2$, $Cl_4C_6O_2C_6Cl_4$
Molecular Weight: 459.751
Melting Point (°C):
  331 (Lide 2003)
Boiling Point (°C):
  510 (Rordorf 1987, 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  229.6, 229.11 (calculated-liquid density, crystalline volume, Govers et al. 1990)
  237.21 (liquid molar volume, Govers et al. 1995)
  344.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  86.7 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
  151.13 (Rordorf 1987)
  145.7 (Li et al. 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  61.4 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  102 (Rordorf 1986,1987,1989; Passivirta et al. 1999)
Fugacity Ratio at 25°C, F: 0.000995 (assuming ΔS_{fus} = 56 J/mol K and mp at 331°C)
  0.00107 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1987)
  0.00115 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)
  3.46×10^{-6} (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  2.0×10^{-6} (Barrie et al. 1983)
  4.0×10^{-7} (^{14}C-labeled, generator column-HPLC/LSC, Webster et al. 1983)
  4.0×10^{-7}* (20°C, ^{14}C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)
  4.0×10^{-7}* (20°C, ^{14}C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Webster et al. 1985)
  1.8×10^{-4} (Opperhuizen 1986)
  1.0×10^{-7} (^{14}C-labeled-LSC, Srinivasan & Fogler 1987)
  7.4×10^{-8}* (extrapolated, generator column-GC/ECD, measured range 40–80°C, Doucette & Andren 1988a)
  $S/(mol/L) = 8.32 \times 10^{-6} \exp(0.041 \cdot t/°C)$ (generator column-GC/ECD, temp range 40–80°C, Doucette & Andren 1988a)
  $\log x = -3891/(T/K) - 1.482$; temp range 40–80°C (generator column-GC/ECD, Doucette & Andren 1988a)
  $\log [S_L/(mol/L)] = -0.163 - 3212/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
  1.03×10^{-4} (supercooled liquid S_L, GC-RI correlation; Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.40×10^{-5}, 1.8×10^{-5} (quoted, calculated-volatilization rate, Dobbs & Cull 1982)
8.70×10^{-6} (20°C, gas saturation, Webster et al. 1985)
1.10×10^{-10}* (gas saturation, Rordorf 1985a,b, 1986a,b, 1987, 1989)
2.51×10^{-10} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf 1986)
2.74×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988)
2.77×10^{-7} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1991)
2.72×10^{-7} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
0.000280* (120.1°C, average value, gas saturation-GC, measured range 120.1–199.7°C, Rordorf 1990)
1.60×10^{-10} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substituted no. plot, Rordorf et al. 1990)
2.62×10^{-10}, 2.56×10^{-10} (solid P_S, calculated from reported P_L, Delle Site 1997)
2.75×10^{-7} (correcting supercooled liquid P_L value of 1988, Eitzer & Hites. 1998)
1.82×10^{-7}; 1.35×10^{-7} (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
2.75×10^{-7}; 4.92×10^{-12} (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P/Pa) = 15.81886 - 7629.38/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.0912* (175°C, Knudsen effusion method, measured range, 175–220°C, Li et al. 2002)
$\log (P_S/Pa) = 13.62 - 7429/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 8.32 - 4221/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
$\ln (P/Pa) = (32.825 \pm 0.153) - (15773 \pm 72)/(T/K)$; temp range 448–493 K (Knudsen effusion method, Li et al. 2002)
6.61×10^{-8} (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)
$\ln (P/Pa) = 38.156 - 16431/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
$\ln (P/Pa) = (36.461 \pm 1.020) - (17529 \pm 487)/(T/K)$; temp range 463–493 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C and the reported temperature dependence equations):
0.683 (calculated-P/C, Shiu et al. 1987,1988)
1.32; 0.513 (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
$\log [H/(Pa\ m^3/mol)] = 8.34 - 1009/(T/K)$ (Passivirta et al. 1999)
0.191; 0.513 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
8.50 (Bruggeman et al. 1984; quoted, Opperhuizen 1986)
12.21, 12.60, 12.97; 11.82, 12.72, 13.08 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
11.16, 12.72 (HPLC-RT correlation, Sarna et al. 1984)
10.56, 7.53 (calculated-TSA, Doucette 1985)
12.26, 11.35; 11.76, 10.07 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
8.60 (HPLC-RT correlation, Burkhard & Kuehl 1986)
7.59 (generator column-GC/ECD, Doucette & Andren 1987)
7.83 (HPLC-RT correlation, Doucette and Andren 1988b)
8.60 (calculated, Endicott & Cook 1994)
7.59, 8.60 (quoted, Hansch et al. 1995)
9.31 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
8.450 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
8.48 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.80 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
13.0 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF:
1.93, 3.35 (fathead minnow; rainbow trout, steady-state, wet weight, Muir et al. 1985,1986)
1.53–2.13; 3.35 (fathead minnow, rainbow trout, Muir et al. 1986)

1.00, 2.05 (human fat, calculated-lipid base, Geyer et al. 1987)
0.903, 1.93 (human fat, calculated-wet wt. base, Geyer et al. 1987)
1.90, 3.10 (guppy: in whole fish, in lipid, Gobas et al. 1987)
6.33; 5.85 (plant parts, calculated-vapor pressure; calculated-vapor pressure & HLC, Reischl et al. 1989)
2.85. 3.97 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990; quoted, Devillers et al. 1996)
2.85 (predicted for biota held in lake enclosures exposed to water concentration of 0.1 ng/g for 0–10 d, Servos et al. 1992b)
2.15 (caged invertebrates exposed to water concn. 2.0 ng/L for 0–10 d, Servos et al. 1992b)
2.32 (caged unionid clams exposed to water concn. 2.9 ng/L for 0–10 d, Servos et al. 1992b)
2.32 (caged white suckers gill exposed to water concn. 2.9 ng/L for 0–10 d, Servos et al. 1992b)
1.89 (caged white suckers carcass exposed to water concn. 1.1 ng/L for 0–10 d, Servos et al. 1992b)
2.42 (caged invertebrates exposed to water concn. 0.6 ng/L for 14–24 d, Servos et al. 1992b)
2.34 (caged unionid clams exposed to water concn. 0.5 ng/L for 14–24 d, Servos et al. 1992b)
2.75 (caged white suckers gill exposed to water concn. 1.3 ng/L for 14–24 d, Servos et al. 1992b)
2.24 (caged white suckers carcass exposed to water concn. 0.4 ng/L for 14–24 d, Servos et al. 1992b)
3.97 (caged white suckers gill exposed to water concn. 2.8 ng/L for 0–104 d, Servos et al. 1992b)
3.95 (caged white suckers carcass exposed to water concn. 2.7 ng/L for 0–104 d, Servos et al. 1992b)
4.13; 3.38 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.13; 4.34; 4.38 (guppy, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from nonlinear regression analysis, Loonen et al. 1994b)
3.38 (*Poecilia reticulata*, quoted, Devillers et al. 1996)
4.13; 4.39 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
7.15, 8.45 (fish 5% lipid: BCF_W, BCF_L, Geyer et al. 2000)
8.02, 7.53 (fish muscle log BCF_L calculated from water, sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
5.92 (estimated DOC partition coeff., Muir et al. 1985)
7.08 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
5.92 (DOC, De Voogt et al. 1990)
7.90 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
10.96; 10.5 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
photolytic $t_{1/2}$ = 16 h by both natural sunlight and fluorescent black light in hexane solution, (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)
solution photolysis $t_{1/2}$ = 1460 min at 1.0 m from a GE Model RS sunlamp and surface photolysis of 46900 min on clean soft glass surface under the same conditions (Nestrick et al. 1980);
photolysis $t_{1/2}$ = 24.3 h in hexadecane solution (Mamantov 1984)
photolysis k = 1.06×10^{-6} s^{-1} in water acetonenitrile (2:3, v/v) solution at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2}$ = 20.53 d in spring; $t_{1/2}$ = 17.85 d in summer; $t_{1/2}$ = 31.26 d in autumn; $t_{1/2}$ = 50.45 d in winter; and $t_{1/2}$ = 863 d averaged over full year (Choudhary & Webster 1986; quoted, Muto et al. 1991)
photolysis rate constant k = 1.06×10^{-6} s^{-1} with $t_{1/2}$ = 183.95 h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: k = 3.45×10^2 d^{-1} with $t_{1/2}$ = 21 d in spring, k = 3.97×10^2 d^{-1} with $t_{1/2}$ = 18 d in summer, k = 2.27×10^2 d^{-1} with $t_{1/2}$ = 31 d in fall, k = 1.40×10^2 d^{-1} with $t_{1/2}$ = 50 d in winter (Choudhary & Webster 1989)
photolysis decay rate constants when irradiated with UV light at 254 nm: k(calc) = 1.77×10^{-5} s^{-1}, 4.62×10^{-5} s^{-1} for fly ash suspensions in distilled water, k(calc) = 1.42×10^{-5} s^{-1} for fly ash suspensions in water-acetonitrile solution (2:3, v/v), and k(calc) = 2.74×10^{-5} s^{-1} for fly ash suspensions in water-acetonitrile solution (2:3, v/v) with ozone (Muto et al. 1991);

photolytic $t_{1/2}$ = 37.3 h-native congener, $t_{1/2}$ = 29.6 h for ^{13}C-labeled congener in extract of fly ash and in tetradecane solution (Tysklind & Rappe 1991);
photolysis $k = 1.6 \times 10^{-3}$ min^{-1} with $t_{1/2}$ = 440 min in pure water, and $k = 1.0 \times 10^{-3}$ min^{-1} with $t_{1/2}$ = 680 min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000);
photodegradation k = 0.12 h^{-1} with $t_{1/2}$ = 5.8 h when loaded on TiO_2 film under UV (λ > 300 nm) or solar light irradiation in the air (Choi et al. 2000)
$t_{1/2}$ = 105 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k (oxidative degradation rate constant of water dissolved OCDD by ozone) is 1.51×10^4 L g^{-1} min^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)
k_{OH}(calc) = 1.6×10^{-12} cm^3 molecule^{-1} s^{-1} and a calculated tropospheric lifetime τ = 9.6 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5×10^6 molecule cm^{-3} for OCDD at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 142 d^{-1}; k_2 = 0.053 d^{-1} (fathead minnow, flow-through system, Muir et al. 1985; quoted, Adams et al. 1986)
k_1 = 11 d^{-1}; k_2 = 0.12 d^{-1} (rainbow trout, flow-through system, Muir et al. 1985)
k_1 = 17, 5.0 d^{-1}; k_2 = 0.103, 0.142 d^{-1} (rainbow trout exposed to concn of 20, 415 ng/L, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)
k_1 = 142 d^{-1}; k_2 = 0.053 d^{-1} (fathead minnow exposed to concn of 9 ng/L, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)
k_2 = 0.046 d^{-1} (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)
k_1 = 984 d^{-1}; k_2 = 1.4 d^{-1} (guppy, Gobas & Schrap 1990)
k_1 = 60 d^{-1}; k_2 = 0.12 d^{-1} (filter-feeder, Servos et al. 1992b)
k_1 = 30 d^{-1}; k_2 = 0.08 d^{-1} (small fish, estimated from Muir et al. 1985 and Servos et at. 1989, Servos et al. 1992b)
k_1 = 275 L kg^{-1} d^{-1}; k_2 = 119 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994)
k_2 = 0.0053 d^{-1} with $t_{1/2}$ = 57 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: atmospheric lifetime of ~7–8 h for reaction with hydroxyl radicals (Atkinson 1987);
estimated reaction k = 0.0015 h^{-1} (Paterson et al. 1990);
photodegradation $t_{1/2}$ = 270 h in a rotary photo-reactor adsorbed to clean silica gels by filtered λ < 290 nm of light (Koester & Hites 1992);
tropospheric lifetime τ = 9.6 d, calculated based on gas-phase reaction with OH radicals (Atkinson 1991);
suggested $t_{1/2}$ = 3950 h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000);
first-order photodegradation k = 0.12 h^{-1} with $t_{1/2}$ = 5.8 h when loaded on TiO_2 film under UV (λ > 300 nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: first order photolytic rate constant k <(0.3– 2.7) × 10^{-3} h^{-1} with $t_{1/2}$ = 7–16 h exposed to sunlight in hexane solution (Dobbs & Grant 1979);
direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2}$ = 20.53 in spring, $t_{1/2}$ = 17.85 d in summer; $t_{1/2}$ = 31.26 d in fall; $t_{1/2}$ = 50.45 d in winter and $t_{1/2}$ = 853.22 d averaged over full year (Choudhary & Webster 1986);
$k = 1.064 \times 10^{-6}$ s^{-1} in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhary & Webster 1985a,1986);
photolysis $t_{1/2}$ = 183.95 h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct photolysis half-lives near water bodies at 40°N latitude: $t_{1/2}$ = 21 d in spring, $t_{1/2}$ = 18 d in summer, $t_{1/2}$ = 31 d in fall and $t_{1/2}$ = 50 d in winter (Choudhary & Webster 1989);
$t_{1/2}$ = 4.0 d in the water column of an experimental lake in northwestern Ontario (Servos et al. 1989);
transformation k(calc) = 1.6×10^{-3} h^{-1} in simulated lake enclosure (Servos et al. 1992a);
photolysis $k = 1.6 \times 10^{-3}$ min^{-1} with $t_{1/2}$ = 440 min in pure water, and $k = 1.0 \times 10^{-3}$ min^{-1} with $t_{1/2}$ = 680 min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000);

suggested $t_{1/2}$ = 79000 h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: estimated reaction k = $(5.0 \times 10^{-3} - 1.0 \times 10^{-6})$ h^{-1} (Paterson et al. 1990);
$t_{1/2}$(calc) = 10 yr with a transformation rate constant k = 7.9×10^{-6} h^{-1} (Servos et al. 1992a)
$t_{1/2}$ = 0.2 – 142 yr (Geyer et al. 2000)
degradation $t_{1/2}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000)
suggested $t_{1/2}$ = 130000 h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).
Soil: undergoes photoreduction on soil surfaces to lower chlorinated congeners (Kieatiwong et al. 1990);
estimated reaction k = 7.0×10^{-7} h^{-1} (Paterson et al. 1990)
$t_{1/2}$ > 10 yr (Geyer et al. 2000)
degradation $t_{1/2}$ = 10–100 yr in soil (estimated, Suzuki et al. 2000)
suggested $t_{1/2}$ = 130000 h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).
Biota: elimination $t_{1/2}$ ~21 d from rat (Norback et al. 1975; quoted, Birnbaum 1985);
elimination $t_{1/2}$ = 13.9 d for fathead minnow (Muir et al. 1985, Adams et al. 1986);
elimination $t_{1/2}$ = 5–13 d for both rainbow trout and fathead minnow (Muir et al. 1986);
mean biological $t_{1/2}$ ~15 d in rainbow trout (Niimi 1986);
$t_{1/2}$ = 15 d in rainbow trout (Niimi & Oliver 1986; quoted, Muir et al. 1986,1990);
$t_{1/2}$ = 57 d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.26.1
Reported aqueous solubilities of octachlorodibenzo-*p*-dioxin at various temperatures

Webster et al. 1985		Friesen et al. 1985		Doucette & Andren 1988a	
generator column-HPLC/LSC		generator column-HPLC/LSC		generator column-GC/ECD	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
20	4.0×10^{-7}	20	4.0×10^{-7}	40	3.11×10^{-7}
40	2.0×10^{-6}	40	2.0×10^{-6}	60	1.82×10^{-6}
				80	7.87×10^{-6}
					$\Delta H_{sol}/(kJ\ mol^{-1})$ = 74.5 at 40–80 °C

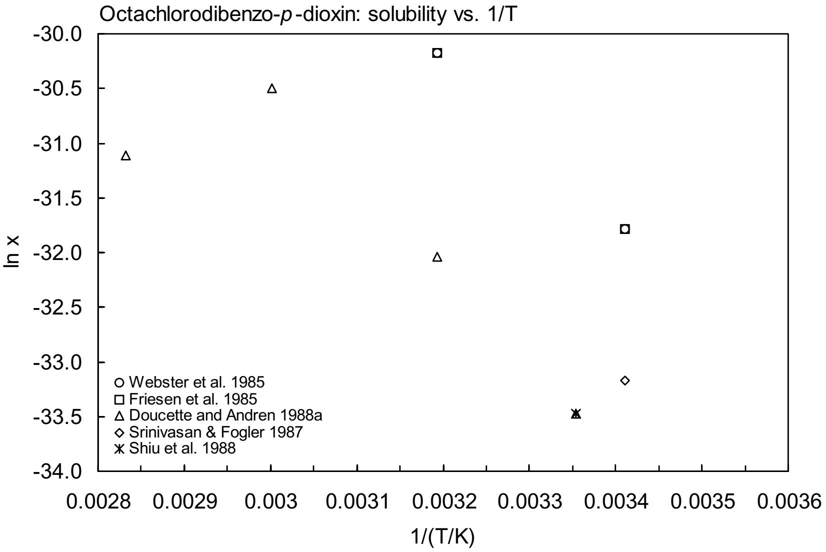


FIGURE 8.1.1.26.1 Logarithm of mole fraction solubility versus reciprocal temperature for octachlorodibenzo-*p*-dioxin.

TABLE 8.1.1.26.2
Reported vapor pressures of octachlorodibenzo-*p*-dioxin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Rordorf 1987, 1989		**Rordorf 1990**		**Li et al. 2002**	
gas saturation-GC		**gas saturation-GC**		**Knudsen effusion**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
			average		
25	1.1×10^{-10}	120.1	0.000280	175	0.0912
50	1.3×10^{-8}	124.9	0.000447	180	0.141
75	7.2×10^{-7}	129.9	0.000737	185	0.204
100	2.4×10^{-5}	134.9	0.00125	190	0.291
125	5.1×10^{-4}	139.9	0.00209	195	0.416
		144.8	0.00352	200	0.607
$\Delta H_V/(kJ\ mol^{-1}) = 86.7$		149.8	0.00581	205	0.838
$\Delta H_{subl}/(kJ\ mol^{-1}) = 151.13$		154.7	0.00949	210	1.20
$\Delta H_{fus}/(kJ\ mol^{-1}) = 61.4$		159.7	0.0153	215	1.67
$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1}) = 102$		165.0	0.0253	220	2.32
		170.0	0.0406		
		175.0	0.0654	eq. 1	P/Pa
		180.0	0.1023	A	32.825
		185.0	0.1585	B	15773
		189.8	0.2515		
		194.7	0.383		
		199.7	0.584		
		$\Delta H_{subl}/(kJ\ mol^{-1}) = 149.822$			
		120 – 200 °C			

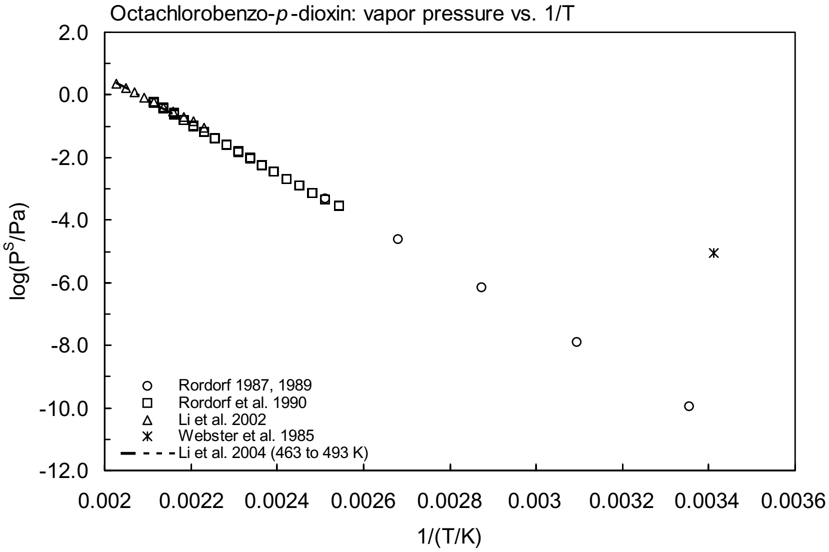


FIGURE 8.1.1.26.2 Logarithm of vapor pressure versus reciprocal temperature for octachlorodibenzo-*p*-dioxin.

8.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 8.2.1
Summary of physical properties of some chlorinated dioxins

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol	
							from $\rho^{(a)}$	Le Bas
Dibenzo-*p*-dioxin	262-12-4	$C_{12}H_8O_2$	184.191	120.5		0.116	143.82	177.0
1-Chloro-	39227-53-7	$C_{12}H_7O_2Cl$	218.636	105.5		0.162	157.41	197.9
2-Chloro-	39227-54-8	$C_{12}H_7O_2Cl$	218.636	89		0.236	154.85	197.9
2,3-Dichloro-	29446-15-9	$C_{12}H_6O_2Cl_2$	253.081	164	358	0.0433	164.07	218.8
2,7-Dichloro-	33857-26-0	$C_{12}H_6O_2Cl_2$	253.081	201	374.5	0.0188	165.88	218.8
2,8-Dichloro-	38964-22-6	$C_{12}H_6O_2Cl_2$	253.081	151		0.0580	165.88	218.8
1,2,4-Trichloro-	39227-58-2	$C_{12}H_5O_2Cl_3$	287.526	129	375	0.0954	179.66	239.7
1,3,7-Trichloro-	67026-17-5	$C_{12}H_5O_2Cl_3$	287.526	148.5	398	0.0614	179.11	239.7
2,3,7-Trichloro-	33857-28-2	$C_{12}H_5O_2Cl_3$	287.526	162–163	408.4	0.0448	175.10	239.7
1,2,3,4-Tetrachloro-	30746-58-8	$C_{12}H_4O_2Cl_4$	321.971	189	419	0.0246	186.71	260.6
1,2,3,7-Tetrachloro-	67028-18-6	$C_{12}H_4O_2Cl_4$	321.971	172	438.3	0.0361	186.52	260.6
1,2,7,8-Tetrachloro-	34816–53–0	$C_{12}H_4O_2Cl_4$	321.971				186.88	260.6
1,3,6,8-Tetrachloro-	30746-58-8	$C_{12}H_4O_2Cl_4$	321.971	219	438.3	0.0125	192.34	260.6
1,3,7,8-Tetrachloro-	50585-46-1	$C_{12}H_4O_2Cl_4$	321.971	193.5–195	438.3	0.0218	188.33	260.6
1,3,7,9-Tetrachloro-	62470-53-5	$C_{12}H_4O_2Cl_4$	321.971				192.34	260.6
2,3,7,8-Tetrachloro-	1746-01-6	$C_{12}H_4O_2Cl_4$	321.971	295		0.00224	184.32	260.6
1,2,3,4,7-Pentachloro-	39227-61-7	$C_{12}H_3O_2Cl_5$	356.416	195	464.7	0.0215	197.74	281.5
1,2,3,7,8-Pentachloro-	40321-76-4	$C_{12}H_3O_2Cl_5$	356.416		464.7		195.74	281.5
1,2,4,7,8-Pentachloro-	58802-08-7	$C_{12}H_3O_2Cl_5$	356.416	206	464.7	0.0168	199.91	281.5
1,2,3,4,7,8-Hexachloro-	39227-26-8	$C_{12}H_2O_2Cl_6$	390.861	273	487.7	0.00369	206.96	302.4
1,2,3,6,7,8-Hexachloro-	57653-85-7	$C_{12}H_2O_2Cl_6$	390.861	285	487.7	0.00281	207.16	302.4
1,2,3,7,8,9-Hexachloro-	19408-74-3	$C_{12}H_2O_2Cl_6$	390.861	243–244	487.7	0.00718	207.16	302.4
1,2,4,6,7,9-Hexachloro-	39227-62-8	$C_{12}H_2O_2Cl_6$	390.861	238–240	487.7	0.00795	215.50	302.4
1,2,3,4,6,7,8-Heptachloro-	35822-46-9	$C_{12}HO_2Cl_7$	425.308	265	507.2	0.00442	218.38	323.3
1,2,3,4,7,8,9-Heptachloro-		$C_{12}HO_2Cl_7$	425.308				222.55	323.3
Octachloro-	3268-87-9	$C_{12}O_2Cl_8$	459.751	331	510	0.000995	229.60	344.2

*Assuming ΔS_{fus} = 56 J/mol K; (a) Govers et al. 1990 (at 25°C).

TABLE 8.2.2
Selected physical-chemical properties of some chlorinated dioxins at 25°C

	Selected properties						Henry's law constant
	Vapor pressure		Solubility				$H/(Pa\cdot m^3/mol)$
Compound	P^S/Pa	P_L/Pa	S/(mg/m³)	C^S/(mmol/m³)	C_L/(mmol/m³)	log K_{OW}	calculated P/C
Dibenzo-*p*-dioxin	0.055	0.474	865	4.696	40.48	4.30	11.71
1-CDD	0.012	0.074	417	1.907	11.77	4.75	6.292
2-CDD	0.017	0.0730	295	1.350	5.717	5.00	12.60
2,3-DCDD	0.00039	0.00901	14.9	0.0589	1.360		6.624
2,7-DCDD	0.00012	0.00811	3.75	0.0148	0.788	6.38	8.098
2,8-DCDD	0.00014	0.00241	16.7	0.0660	1.138		2.122
1,2,4-T_3CDD	0.0001	0.00105	8.41	0.0293	0.306		3.419
1,2,3,4-T_4CDD	6.40×10^{-6}	2.60×10^{-4}	0.55	0.0017	0.0694	6.60	3.747
1,2,3,7-T_4CDD	1.00×10^{-6}	2.77×10^{-5}	0.42	0.0013	0.0361	6.90	0.766
1,3,6,8-T_4CDD	7.00×10^{-7}	5.60×10^{-5}	0.32	0.000994	0.0795	7.18	0.704
2,3,7,8-T_4CDD	2.00×10^{-7}	8.93×10^{-5}	0.0193	0.00006	0.0268	6.80	3.336
1,2,3,4,7-P_5CDD	8.80×10^{-8}	4.09×10^{-6}	0.118	0.000331	0.0154	7.40	0.266
1,2,3,4,7,8-H_6CDD	5.10×10^{-9}	1.38×10^{-6}	0.006	1.54×10^{-5}	0.00416	7.80	0.332
1,2,3,4,6,7,8-H_7CDD	7.50×10^{-10}	1.70×10^{-7}	0.0024	5.64×10^{-6}	0.00128	8.00	0.133
OCDD	1.10×10^{-10}	1.11×10^{-7}	0.000074	1.61×10^{-7}	0.00016	8.20	0.683

TABLE 8.2.3
Suggested half-life classes of polychlorinated dibenzo-*p*-dioxins in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Dibenzo-*p*-dioxin	3	3	6	7
2-CDD	4	4	7	8
2,7-DCDD	4	4	7	8
2,8-DCDD	4	4	7	8
1,2,4-T_3CDD	4	4	7	8
1,2,3,4-T_4CDD	4	5	8	9
2,3,7,8-T_4CDD	4	5	8	9
1,2,3,4,7-P_5CDD	5	5	8	9
1,2,3,4,7,8-H_6CDD	5	6	9	9
1,2,3,4,6,7,8-H_7CDD	5	6	9	9
OCDD	5	7	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55888 (~ 6 years)	> 30,000

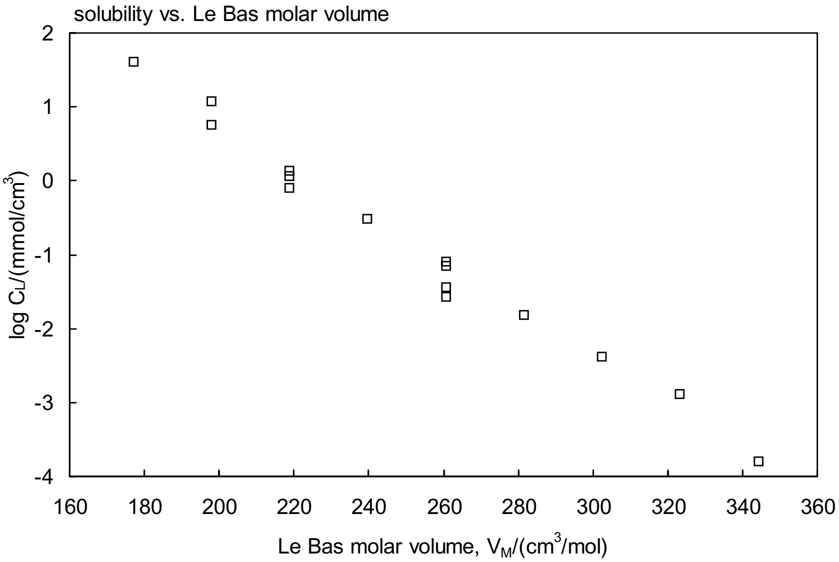


FIGURE 8.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

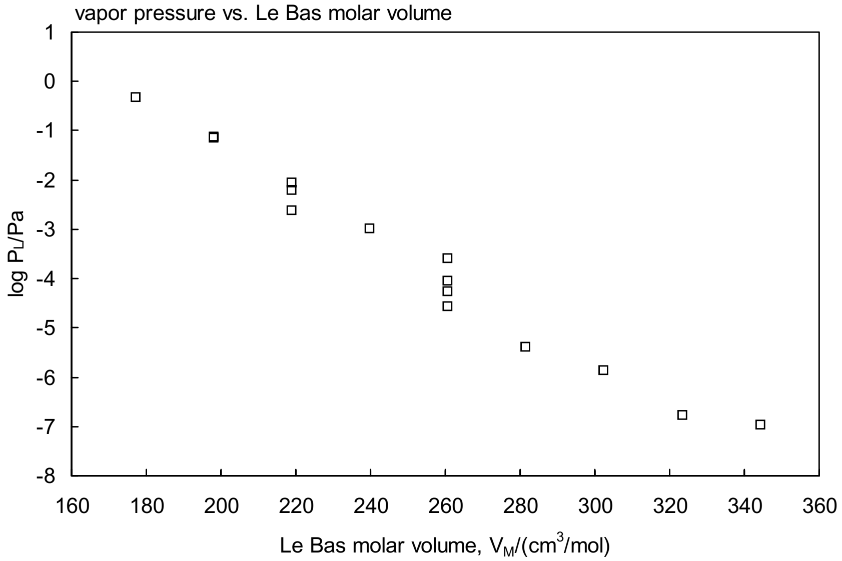


FIGURE 8.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

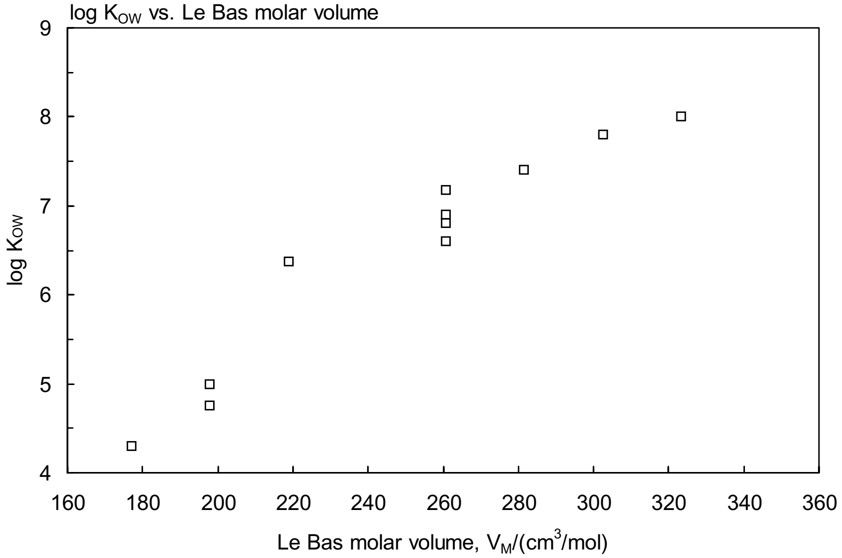


FIGURE 8.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

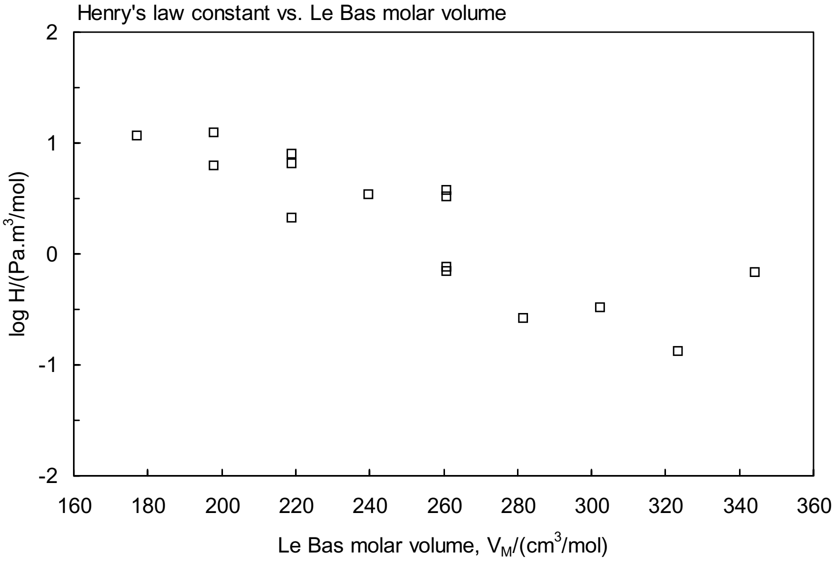


FIGURE 8.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

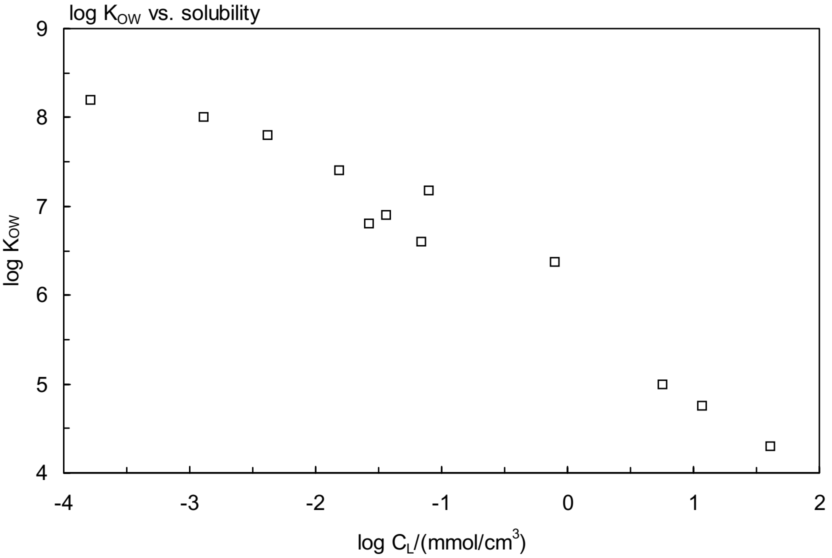


FIGURE 8.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated dibenzo-*p*-dioxins.

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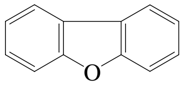
9 Chlorinated Dibenzofurans

CONTENTS

9.1 LIST OF CHEMICALS AND DATA COMPILATIONS

9.1.1 DIBENZOFURAN AND CHLORINATED DIBENZOFURANS

9.1.1.1 Dibenzofuran



Common Name: Dibenzofuran
Synonym: diphenylene oxide
Chemical Name: dibenzofuran
CAS Registry No: 132-64-9
Molecular Formula: $C_{12}H_8O$, $C_6H_4OC_6H_4$
Molecular Weight: 168.191
Melting Point (°C):
86.5 (Lide 2003)
Boiling Point (°C):
287 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 20°C):
1.0886 (99°C, Weast 1982–83)
Molar Volume (cm^3/mol):
154.4 (99°C, calculated-density, Stephenson & Malanowski 1987)
147.8 (Ruelle & Kesselring 1997)
176.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
65.4 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
85.63 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.6 (Rordorf 1987, 1989; quoted, Ruelle & Kesselring 1997)
18.6 (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
54 (Rordorf 1986, 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.249 (mp at 86.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3.11 (Lu et al. 1978)
10.03 (shake flask-HPLC/UV, Banerjee et al. 1980)
6.56 (selected average, Pearlman et al. 1984)
4.22* (generator column-GC, measured range 4–39.8°C, Doucette & Andren 1988a)
$S/(mol/L) = 8.32 \times 10^{-6} \exp(0.041 \cdot t/°C)$; temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a); or
$\log x = -1558/(T/K) - 1.135$; temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
3.36 (calculated-TSA, Dickhut et al. 1994)
4.30 (computed-expert system SPARC, Kollig 1995)
4.75* ± 0.22 (generator column-HPLC/UV, Shiu et al. 1997)
4.69 ± 0.18 (shake flask-GC, Shiu et al. 1997)
2.43 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle Kesselring 1997)
17.21; 62.49 (supercooled liquid S_L, quoted lit. average; calculated-SOFA-Solubility parameters for Fate Analysis model, Govers & Krop 1998)
$\ln x = -1.6385 - 3842.2/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.276* (gas saturation, extrapolated-Antoine eq. from exptl. data, measured temp range, 30–70°C, Hansen & Eckert 1986)
0.506* (26°C, gas saturation exptl. data, measured range 49–74°C, Sato et al. 1986)
0.466 (gas saturation-GC, extrapolated-Antoine eq. derived from exptl. data, temp range 49–74°C, Sato et al. 1986)
0.35* (gas saturation-GC, measured range 25–125°C Rordorf 1986, 1989)
2.026 (extrapolated liquid value P_L, Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 5.8968 - 1851.27/(-82.64 + T/K)$; temp range 403–559 K (Antoine eq., Stephenson & Malanowski 1987)
0.40 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
$\log (P/mmHg) = 17.6646 - 3.1989 \times 10^3/(T/K) - 3.3346 \cdot \log(T/K) + 6.0686 \times 10^{-10} \cdot (T/K) + 4.4676 \times 10^{-7} \cdot (T/K)^2$; temp range 356–838 K (vapor pressure eq., Yaws et al. 1994)
0.360 (computed-expert system SPARC, Kollig 1995)
0.708; 0.123 (supercooled liquid P_L, quoted exptl. or exptl. average; calculated-SOFA model (Solubility parameters of Fate Analysis model), Govers & Krop 1998)
$\log (P/Pa) = 13.17192 - 4083/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.429 (gas saturation-HPLC/fluorescence, de Seze et al. 2000)
0.398* (25.2°C, Knudsen effusion method, measured range 20.2–45°C Li et al. 2002)
$\ln (P/Pa) = 33.54 - 10313/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2002 2004)
$\ln (P/Pa) = (32.203 \pm 0.576) - (9880.4 \pm 176)/(T/K)$; temp range 295–318 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):

14.16 (calculated-P/C with selected values)
14.20 (computed-expert system SPARC, Kollig 1995)
21.38, 13.80 (calculated-P/C, Govers & Krop 1998)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.12 (HPLC-RT correlation, Veith et al. 1979a)
4.12 (Hansch & Leo 1979)
4.17 (shake flask-HPLC/UV, Banerjee et al. 1980)
3.91, 4.12, 4.18; 3.96, 4.10, 4.17 (HPLC-RT, linear regressions; quadratic regressions, Sarna et al. 1984)
3.92 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
4.31 (generator column-GC/ECD, both phases, Doucette & Andren 1987)
3.86 (HPLC-RT correlation, Doucette & Andren 1988b)
4.21, 3.81 (shake flask-HPLC, TLC-RT correlation, De Voogt et al. 1990)
4.12 (recommended, Sangster 1993)
4.12 (recommended, Hansch et al. 1995)
4.27 (generator column-HPLC/UV, Shiu et al. 1997)
4.273* (shake flask-HPLC/UC, measured S_O and S_W, Shiu et al. 1997)
4.09 ± 0.19, 4.12 ± 0.63; 4.12 (HPLC-k′ correlation: ODS-65 column, Diol-35 column; quoted lit average value, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

3.13 (fathead minnow, 28 d exposure, Veith et al. 1979b)
3.13, 2.80 (quoted exptl., calculated-K_{OW}, Mackay 1982)
3.13, 3.13 (quoted exptl., calculated-MCI χ, Sabljic 1987)

3.13 (calculated-K_{OW}, Isnard & Lambert 1989)
3.68; 4.08 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:
3.80 (computed-K_{OW}, Kollig 1995)
4.15 (humic acid, HPLC-k′ correlation, Nielsen et al. 1997)
3.45 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
3.84 (soil-pore-water partition coeff. for Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = 3.4 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} corresponding to an atmospheric lifetime of about 8 h (Atkinson 1987a)
$k_{OH} = 3.3 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (Atkinson 1987b)
$t_{½}$ = 1.9–19 h based on estimated rate constant with OH radicals in air (Howard 1991)
$k_{OH} = 31 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} the tropospheric lifetime was calculated to be 0.5 d (Atkinson 1991)
$k_{OH} = 3.9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and with calculated tropospheric lifetime of 3.7 d; $k_{NO3} < 7 \times 10^{-30}$ cm^3 molecule^{-1} s^{-1} with calculated tropospheric lifetime >7 yr and $k_{O3} < 8 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} with O_3 with calculated tropospheric lifetime >250 d at room temp. (Kwok et al. 1994)
k_{OH}(exptl) = 3.9×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(calc) = 7.0×10^{-12} cm^3 molecule^{-1} s^{-1} corresponding to a tropospheric lifetime of 3.7 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation: biodegradation $t_{½}$ ~168–672 h and anaerobic $t_{½}$ = 672–2688 h, based on aerobic acclimated and unacclimated groundwater die-away test data (Lee et al. 1984; quoted, Ward et al. 1986; Howard et al. 1991);
nonautoclaved groundwater samples at hazardous waste site with a concentration of approximate 0.09 mg/L are degraded by microbes at rates about 30% per week while the levels of the controls decreased only about half that rate (Lee et al. 1984).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: the calculated atmospheric lifetime range from ~60–120 h (Atkinson 1987a);
$t_{½}$ = 1.9–19 h, based on estimated rate constants for reaction with OH radicals (Howard et al. 1991);
the tropospheric lifetime was calculated 0.5 d for the gas-phase reaction for OH radicals using a 12-h average daytime OH radical concn of 1.5×10^6 (Atkinson 1991);
calculated room temp. tropospheric lifetimes of 3.7 d for reaction with OH radical, >7 yr with NO_3 radical, and >250 d for reaction with O_3 (Kwok et al. 1994);
room temp. tropospheric lifetime was calculated to be 3.7 d for reaction with OH radical (Kwok et al. 1995).
Surface water: $t_{½}$ =168–672 h, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).
Groundwater: $t_{½}$ = 205–835 h, based on aerobic acclimated and unacclimated groundwater die-away teat data (Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 168–672 h, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).
Biota:

TABLE 9.1.1.1
Reported aqueous solubilities and octanol-water partition coefficients of dibenzofuran at various temperatures

Aqueous solubility				Octanol-water partition coefficient	
Shiu et al. 1997		Doucette & Andren 1988a		Shiu et al. 1997	
generator column-HPLC/UV		generator column-GC/ECD		generator column-HPLC/UV	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$\log K_{OW}$
5	1.914	3.9	1.652	5	4.405
15	3.004	25	4.222	15	4.346
25	4.75	39.8	6.963	25	4.273
35	7.56			35	4.190
45	11.8	$\Delta H_{sol}/(kJ\ mol^{-1}) = 29.8$		45	4.116
		for 4–32°C			
shake flask-HPLC/UV				$\Delta H/(kJ\ mol^{-1}) = -12.4$	
25	4.69				
$\Delta H_{sol}/(kJ\ mol^{-1}) = 33.3$					
5–45°C					

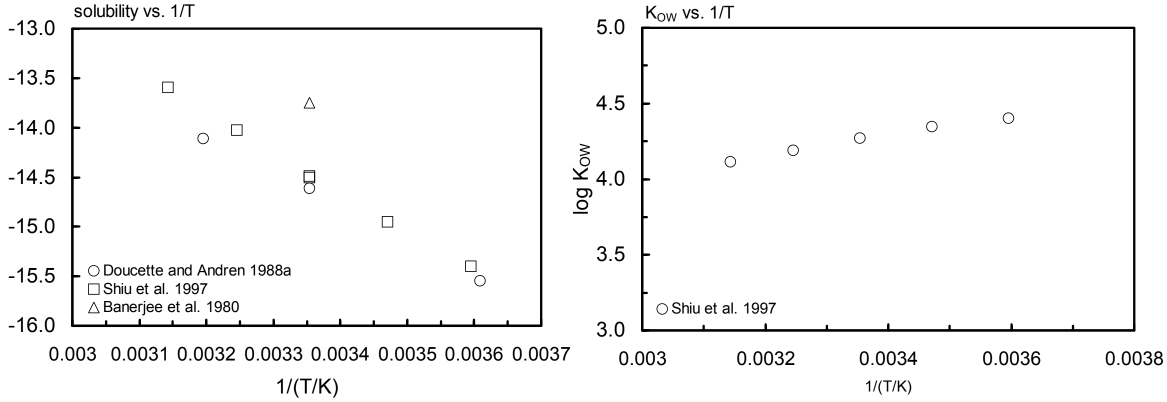


FIGURE 9.1.1.1 Logarithm of mole fraction solubility and K_{OW} versus reciprocal temperature for dibenzofuran.

TABLE 9.1.1.2
Reported vapor pressures of dibenzofuran at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Hanson & Eckert 1986		Sato et al. 1986		Rordorf 1989		Li et al. 2002	
gas saturation-IR		gas saturation-electrobalance		gas saturation-GC		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30	0.4874	25.85	0.506	25	0.35	20.2	0.284
35	0.7818	35.85	1.48	50	5.10	25.2	0.398
40	1.280	40.75	2.35	75	50.0	30	0.665
45	2.128	45.85	3.71	100	360	35	1.22
50	3.200	52.45	6.69	125	2100	40	1.94
55	4.679	55.65	8.8			45	3.04
60	7.246	59.75	12.5	$\Delta H_V/(kJ\ mol^{-1}) = 65.4$			
65	12.78	60.35	13.5	$\Delta H_{subl}/(kJ\ mol^{-1}) = 85.630$		eq. 1	P/Pa
70	19.71	64.45	18.3	$\Delta H_{fus}/(kJ\ mol^{-1}) = 19.6$		A	32.203
		65.05	19.9	$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1}) = 54$		B	9880.4
log (P/mPa) = B – A/(T/K)		66.15	21.5				
A	16.30	68.75	26.1				
B	4132	69.35	27.1				
$\Delta H_{subl}/(kJ\ mol^{-1}) = 79.1$		72.75	35.4				
		eq. 3	P/Pa				
		A	22.1098				
		B	4707.68				
		C	–92.332				

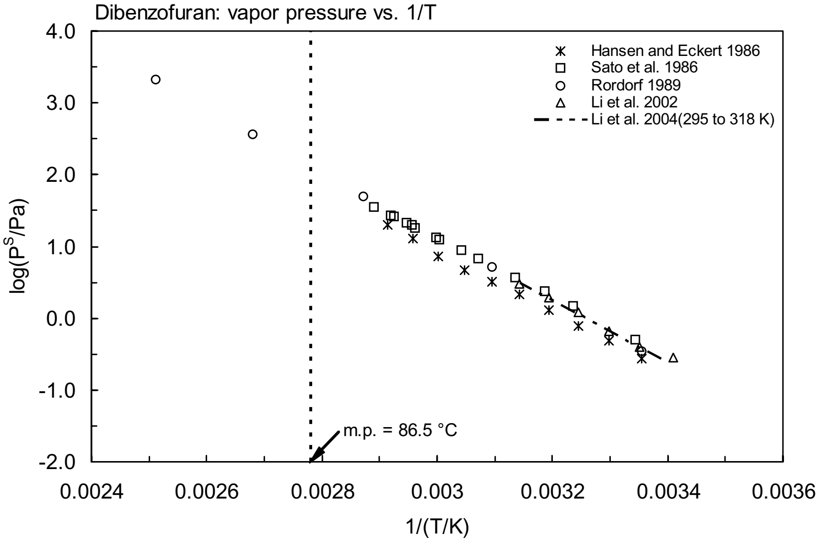
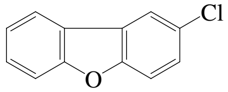


FIGURE 9.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for dibenzofuran.

9.1.1.2 2-Chlorodibenzofuran



Common Name: 2-Chlorodibenzofuran
Synonym: 2-MCDF
Chemical Name: 2-Chlorodibenzofuran
CAS Registry No: 51230-49-0
Molecular Formula: $C_{12}H_7ClO$, $C_6H_4OC_6H_3Cl$
Molecular Weight: 202.637
Melting Point (°C):
101.5–102.5 (Rordorf 1989)
Boiling Point (°C):
338.2 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
197.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
75.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
95.28 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.4 (Rordorf 1987, 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
52 (Rordorf 1986, 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
11.66 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
4.23, 11.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
9.6×10^{-3}, 0.190, 2.40, 22.0, 150 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
0.537 (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
$\log (P_L/\text{mmHg}) = 40.57 - 5556/(T/K) - 9.999\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
0.174; 0.537 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
9.12 (calculated-SOFA model, Govers & Krop 1998)
10.23; 9.12 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
4.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
5.15; 4.37 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
4.51 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
4.77; 4.51 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

4.38	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
3.96; 4.38	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (16–22) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for a mono-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 0.7–1.0 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = (5.0–5.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and the calculated tropospheric lifetime was 2.9 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a mono-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 0.7–1.0 d (Atkinson 1991);

calculated tropospheric lifetime was 2.9 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

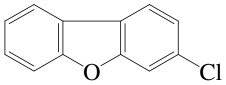
Ground water:

Sediment:

Soil:

Biota:

9.1.1.3 3-Chlorodibenzofuran



Common Name: 3-Chlorodibenzofuran
Synonym: 3-MCDF
Chemical Name: 3-Chlorodibenzofuran
CAS Registry No: 25074-67-3
Molecular Formula: $C_{12}H_7ClO$, $C_6H_4OC_6H_3Cl$
Molecular Weight: 202.637
Melting Point (°C):
101–102 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
338.2 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
197.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
75.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
95.313 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.4 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
52 (Rordorf 1986, 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
12.21 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
6.34; 12.21 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.970, 0.190, 2.40, 22.0, 150 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
0.490 (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
$\log (P_L/\text{mmHg}) = 40.57 - 5553/(T/K) - 9.999\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
0.174; 0.490 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
7.76 (calculated-SOFA model, Govers & Krop 1998)
10.23; 7.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
4.35 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
5.15; 4.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
4.53 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
4.77; 4.53 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

4.34	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
3.96; 4.34	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (16–22) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for a mono-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 0.7–1.0 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = (5.0–5.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and the calculated tropospheric lifetime was 2.9 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a mono-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 0.7–1.0 d (Atkinson 1991);
calculated tropospheric lifetime of 2.9 d for with OH radical (Kwok et al. 1995).

Surface water:

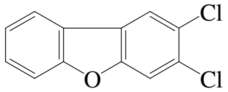
Ground water:

Sediment:

Soil:

Biota:

9.1.1.4 2,3-Dichlorodibenzofuran



Common Name: 2,3-Dichlorodibenzofuran
Synonym: 2,3-DCBF
Chemical Name: 2,3-dichlorodibenzofuran
CAS Registry No: 64126-86-9
Molecular Formula: $C_6H_3ClOC_6H_3Cl$
Molecular Weight: 237.082
Melting Point (°C):
 125.5–127 (Rordorf 1989)
Boiling Point (°C):
 375 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
 218.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 78.8 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
 105.04 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 25.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 63 (Rordorf 1986, 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
 1.50 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
 0.716; 1.50 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 6.50×10^{-4}, 1.7×10^{-2}, 0.29, 3.20, 27.0 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
 0.0282 (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
 $\log (P_L/\text{mmHg}) = 39.20 - 5757/(T/K) - 9.466\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 0.1096; 0.0282 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
 4.365 (calculated-SOFA model, Govers & Krop 1998)
 4.79; 4.365 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
 5.11 (calculated-SOFA model, Govers & Krop 1998)
 5.43; 5.11 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
 4.82 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
 5.04; 4.82 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

5.39	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
5.15; 5.39	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (6.6–16) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = (2.6–3.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 0.7–1.0 d (Atkinson 1991);

room temp. tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical (Kwok et al. 1995).

Surface water:

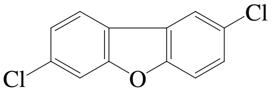
Ground water:

Sediment:

Soil:

Biota:

9.1.1.5 2,7-Dichlorodibenzofuran



Common Name: 2,7-Dichlorodibenzofuran
Synonym: 2,7-DCBF
Chemical Name: 2,7-dichlorodibenzofuran
CAS Registry No: 73992-98-6
Molecular Formula: $C_6H_3ClOC_6H_3Cl$
Molecular Weight: 237.082
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
  218.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
  2.32 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
  0.785; 2.32 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  0.0501 (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
  $\log (P_L/\text{mmHg}) = 39.23 - 5755/(T/K) - 9.466 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
  0.0123; 0.0501 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol):
  5.01 (calculated-SOFA model, Govers & Krop 1998)
  4.90; 5.01 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
  5.02 (calculated-SOFA model, Govers & Krop 1998)
  5.41; 5.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
  4.79 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
  5.03; 4.79 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:
  5.27 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
  5.10; 5.27 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
  Volatilization:
  Photolysis: photolysis k = 0.23 min^{-1} with $t_{1/2}$ = 3.0 min in pure water and k = 0.011 min^{-1} with $t_{1/2}$ = 63 min in 60 % acetonitrile/water solution in Corex centrifuge bottles at 300 nm photochemical reactor (Kim & O'Keefe 2000)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (6.6–16) × 10^{-12} cm^3 molecule^{-1} s^{-1} for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = (2.6–3.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 0.7–1.0 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical at room temp. (Kwok et al. 1995).

Surface water:

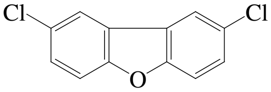
Ground water:

Sediment:

Soil:

Biota:

9.1.1.6 2,8-Dichlorodibenzofuran



Common Name: 2,8-Dichlorodibenzofuran
Synonym: 2,8-DCDF
Chemical Name: 2,8-dichlorodibenzofuran
CAS Registry No: 5409-83-6
Molecular Formula: $C_6H_3ClOC_6H_3Cl$
Molecular Weight: 237.082
Melting Point (°C):
184–185 (Kuroki et al. 1984)
Boiling Point (°C):
375 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
218.5 (calculated-Le Bas method at normal boiling point)
173.6 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
74.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
101.423 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
25.1 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
18.6 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
55 (Rodorf 1989)
Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0145* (generator column-GC, measured range 4.5–39.5°C, Doucette & Andren 1988a)
$S/(mol/L) = 1.24 \times 10^{-6} \exp(0.082 \cdot t/°C)$ (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
$\log x = -2344/(T/K) - 1.093$; temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
0.024 (calculated-TSA, Dickhut et al. 1994)
0.0431 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
2.11 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
$\ln x = -2.515 - 5398.4/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.75; 2.11 (supercooled liquid S_L, GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
9.6×10^{-4} (estimated, van den Berg & Olie 1985)
3.9×10^{-4}* (calculated-bp and ΔH_{fus}, Rordorf 1987, 1989)
0.0145; 0.0417 (supercooled liquid P_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
$\log (P/Pa) = 14.30669 - 5281.67/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.0115; 0.0417 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
1.06×10^{-3} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
0.0412 (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
$\log (P_L/mmHg) = 39.21 - 5756/(T/K) - 9.466 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

ln (P/Pa) = 32.943 – 12162/(T/K), temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
ln (P/Pa) = (36.010 ± 0.393) – (13262 ± 144)/(T/K); temp range 348–383 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):

6.31; 4.57	(quoted lit.; calculated-SOFA model, Govers & Krop 1998)
4.79; 4.57	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

5.56, 5.97, 6.16; 5.65, 5.95, 6.15 (HPLC-RT correlation, linear regressions; quadratic regressions, Sarna et al. 1984)

5.30	(re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
5.44	(generator column-GC/ECD, Doucette & Andren 1987)
5.12	(HPLC-RT correlation, Doucette & Andren 1988b)
5.65	(recommended, Sangster 1993)
5.65	(recommended, Hansch et al. 1995)
5.42	(GC-RI correlation; Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

5.04	(guppy, Loonen et al. 1994a)
5.04; 4.81	(lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
5.04; 4.81	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

5.30	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
5.13; 5.30	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: when 5 mg/L in methanol was irradiated by sunlight simulator more than 95% disappears within 48 h while a similar experiment with highly purified methanol solution reveals only very slow photolysis within the same period of irradiation and results were same with 10 mg/L in methanol solution (Crosby & Moilanen 1973; quoted, Choudhary & Hutzinger 1982);

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (6.6–16) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = (2.6–3.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 1.0–2.3 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radicals (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:
Biota: mean biological $t_{1/2}$ ~ 11 d in rainbow trout (Niimi 1986).

TABLE 9.1.6.1
Reported aqueous solubilities and vapor pressures of 2,8-dichlorodibenzofuran at various temperatures

Aqueous solubility		Vapor pressure	
Doucette & Andren 1988a		Rordorf 1989	
generator column-GC/ECD		vapor pressure correlation	
t/°C	S/g·m^{-3}	t/°C	P/Pa
4.5	0.00384	25	3.9×10^{-4}
25	0.0145	50	9.1×10^{-3}
39.5	0.0339	75	0.14
		100	1.40
ΔH_{sol}/(kJ mol^{-1})		125	11.0
4–32°C	44.9		
		ΔH_V/(kJ mol^{-1}) = 74.2	
S/(mol/L) = a·exp[b·(t/°C)]		ΔH_{subl}/(kJ mol^{-1}) = 101.423	
a	1.24×10^{-8}	ΔH_{fus}/(kJ mol^{-1}) = 25.1	
b	0.062	ΔS_{fus}/(J mol^{-1} K^{-1}) = 55	

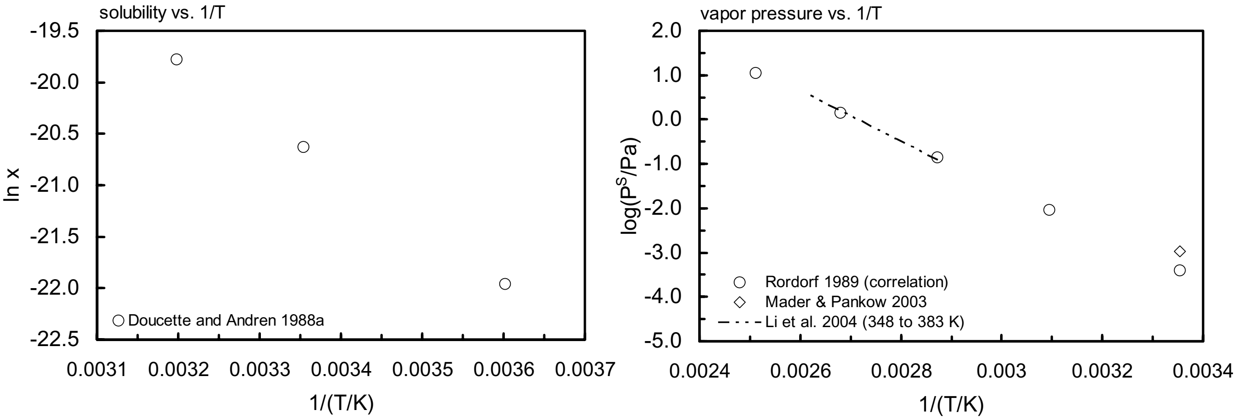
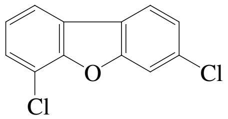


FIGURE 9.1.6.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,8-dichlorodibenzofuran.

9.1.1.7 3,6-Dichlorodibenzofuran



Common Name: 3,6-Dichlorodibenzofuran
Synonym: 3,6-DCDF
Chemical Name: 3,6-dichlorodibenzofuran
CAS Registry No: 94570-83-9
Molecular Formula: $C_6H_3ClOC_6H_3Cl$
Molecular Weight: 237.082
Melting Point (°C):
 188 (Rordorf 1989)
Boiling Point (°C):
 357 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
 218.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 70.7 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
 110.87 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 38.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 83 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0252 (mp at 188°C)

Water Solubility (g/m^3 or mg/L at 25°C):
 1.76 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
 0.684; 1.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 2.0×10^{-4}, 6.3×10^{-3}, 0.12, 1.60, 15 (25, 50, 75, 100, 125°C, gas saturation-GC, Rordorf 1985a,b, 1987, 1989)
 0.0355 (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
 0.0123; 0.0355 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
 $\log (P_L/\text{mmHg}) = 39.18 - 5755/(T/K) - 9.466 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
 4.57 (calculated-SOFA model, Govers & Krop 1998)
 4.68; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
 5.08 (calculated-SOFA model, Govers & Krop 1998)
 5.44; 5.08 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
 4.81 (lipid wt. basis, calculated-SOFA model, Govers & Krop 1998)
 5.05; 4.81 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

5.35	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
5.18; 5.35	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (6.6–16) × 10^{-12} cm^3 molecule^{-1} s^{-1} for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = (2.6–3.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 1.0–2.3 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical (Kwok et al. 1995).

Surface water:

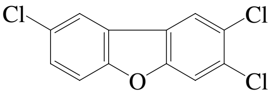
Ground water:

Sediment:

Soil:

Biota: mean biological $t_{1/2}$ = 24 d in rainbow trout (Niimi & Oliver 1986)

9.1.1.8 2,3,8-Trichlorodibenzofuran



Common Name: 2,3,8-Trichlorodibenzofuran
Synonym: 2,3,8-TCDF
Chemical Name: 2,3,8-trichlorodibenzofuran
CAS Registry No: 57117-32-5
Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$
Molecular Weight: 271.527
Melting Point (°C):
  189–191 (Rordorf 1989)
Boiling Point (°C):
  408.4 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
  239.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  70.8 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
  111.823 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  30.9 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  67 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
  0.291 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
  0.113, 0.291 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  3.0×10^{-5}, 9.9×10^{-4}, 2.0×10^{-2}, 0.26, 2.50 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
  4.27×10^{-3} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
  9.12×10^{-4}, 4.27×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
  2.48×10^{-4} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
  0.0108 (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
  $\log (P_L/\text{mmHg}) = 37.66 - 5911/(T/K) - 8.932 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  3.24 (calculated-SOFA model, Govers & Krop 1998)
  2.57; 3.24 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
  5.76 (calculated-SOFA model, Govers & Krop 1998)
  5.75; 5.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

4.94	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.20; 4.94	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

6.30	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.26; 6.30	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (3.4–12) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for a tri-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.3–4.5 d using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = $(1.5–2.6) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and the calculated tropospheric lifetime was 5.5–9.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991);

calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

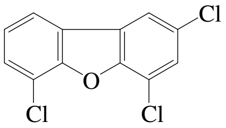
Ground water:

Sediment:

Soil:

Biota:

9.1.1.9 2,4,6-Trichlorodibenzofuran



Common Name: 2,4,6-Trichlorodibenzofuran
Synonym: 2,4,6-PCDF
Chemical Name: 2,4,6-trichlorodibenzofuran
CAS Registry No: 58802-14-6
Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$
Molecular Weight: 271.527
Melting Point (°C):
116–117 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
408.4 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
239.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
84.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
116.061 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
30.9 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
79 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.461 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.175; 0.461 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
5.33×10^{-4} (estimated, Van den Berg & Olie 1985)
8.2×10^{-5}, 3.1×10^{-3}, 6.8×10^{-2}, 1.0, 10.0 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
4.27×10^{-3} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
1.32×10^{-3}, 4.27×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
9.22×10^{-4} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
7.50×10^{-3} (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
$\log (P_L/\text{mmHg}) = 37.77 - 5908/(T/K) - 8.932 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
$\ln (P/\text{Pa}) = 37.264 - 13912/(T/K)$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
$\ln (P/\text{Pa}) = (35.837 \pm 0.729) - (13090 \pm 259)/(T/K)$; temp range 338–373 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa·m^3/mol at 25°C):
2.40 (calculated-SOFA model, Govers & Krop 1998)
2.82; 2.40 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
5.64 (calculated-SOFA model, Govers & Krop 1998)
5.69; 5.64 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

4.99	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.18; 4.99	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

6.12	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.09; 6.12	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (3.4 – 4.8) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (3.4 – 12) × 10^{-12} cm^3 molecule^{-1} s^{-1} with calculated tropospheric lifetime of 1.3–4.5 d, using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3 for a tri-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k_{OH}(calc) = (1.5 – 2.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} with a calculated lifetime of 4.0–5.5 d for a tri-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991); calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical for a tri-chlorinated dibenzofuran (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

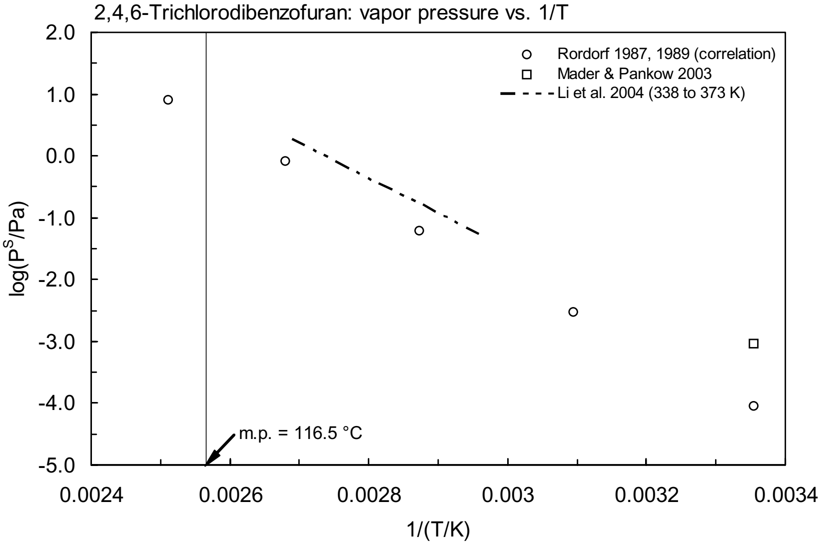
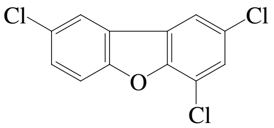


FIGURE 9.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trichlorodibenzofuran.

9.1.1.10 2,4,8-Trichlorodibenzofuran



Common Name: 2,4,8-Trichlorodibenzofuran
Synonym: 2,4,8-TCDF
Chemical Name: 2,4,8-trichlorodibenzofuran
CAS Registry No: 54589-71-8
Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$
Molecular Weight: 271.527
Melting Point (°C):
155–156 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
392.5 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
239.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
78.7 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
112.3 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
32.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
76 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0542 (mp at 154°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.494 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.157; 0.494 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
9.1×10^{-5}* (gas saturation-GC, Rordorf 1989)
5.75×10^{-3} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
$\log (P_L/\text{mmHg}) = 37.78 - 5809/(T/K) - 8.932 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
1.38×10^{-3}, 5.75×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
3.09 (calculated-SOFA model, Govers & Krop 1998)
2.88; 3.09 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
5.64 (calculated-SOFA model, Govers & Krop 1998)
5.69; 5.64 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
4.94 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.18; 4.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Sorption Partition Coefficient, log K_{OC}:

6.14	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.06; 6.14	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
  k_{OH} = (3.4–12) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for a tri-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.3–4.5 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)
  k_{OH}(calc) = (1.5–2.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and the calculated tropospheric lifetime was 5.5–9.5 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991);
  calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:

TABLE 9.1.10.1
Reported vapor pressures of 2,4,8-tetrachlorodibenzofuran at various temperatures

Rordorf 1987, 1989	
gas saturation-GC	
t/°C	**P/Pa**
25	9.1×10^{-5}
50	3.0×10^{-3}
75	6.1×10^{-2}
100	0.82
125	8.0
$\Delta H_V/(kJ\ mol^{-1})$ = 78.7	
$\Delta H_{subl}/(kJ\ mol^{-1})$ = 112.3	
$\Delta H_{fus}/(kJ\ mol^{-1})$ = 32.6	
$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1})$ = 76	

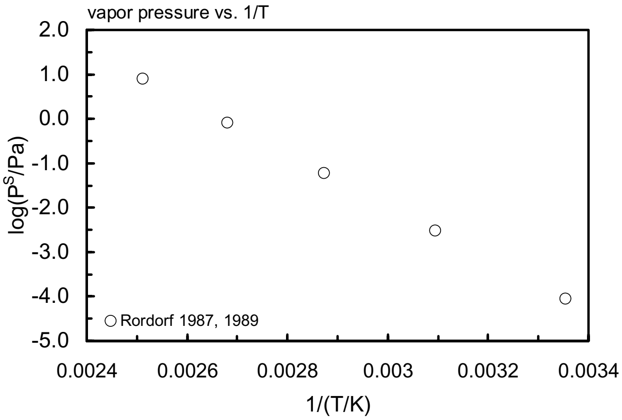
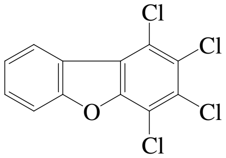


FIGURE 9.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,8-trichlorodibenzofuran.

9.1.1.11 1,2,3,4-Tetrachlorodibenzofuran



Common Name: 1,2,3,4-Tetrachlorodibenzofuran
Synonym: 1,2,3,4-TCDF
Chemical Name: 1,2,3,4-tetrachlorodibenzofuran
CAS Registry No: 24478-72-6
Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$
Molecular Weight: 305.978
Melting Point (°C):
168.5–169 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
438.3 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
260.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
84.4 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
122.826 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
83 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0717 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0306; 0.0717 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
4.1×10^{-6}, 1.9×10^{-4}, 5.1×10^{-3}, 8.7×10^{-2}, 1.0 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
6.76×10^{-4} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
$\log (P_L/\text{mmHg}) = 36.02 - 6019/(T/K) - 8.399 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
1.17×10^{-4}, 6.76×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
2.75 (calculated-SOFA model, Govers & Krop 1998)
1.74; 2.75 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.17 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)
6.34 (calculated-SOFA model, Govers & Krop 1998)
6.07; 6.34 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

4.92	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.22; 4.92	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

7.12	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.18; 7.12	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: sunlight induced photolysis $t_{½}$ = 220 min in isooctance solution, and solid phase photolysis half-life, $t_{½}$ = 95 h with PCDF dispersed as solid films (Buser 1988)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (1.4–8.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = (0.8–1.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 154, 134 L kg^{-1} d^{-1}; k_2 >1.8, >1.4 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 171 L kg^{-1} d^{-1}, 220 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3}, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991);

calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

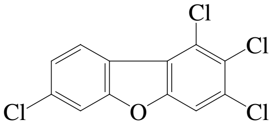
Ground water:

Sediment: degradation $t_{½}$ = 20–200 yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: half-lives in gold fish: $t_{½}$ < 0.4 d for PBO treated and $t_{½}$ > 0.5 d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.12 1,2,3,7-Tetrachlorodibenzofuran



Common Name: 1,2,3,7-Tetrachlorodibenzofuran
Synonym: 1,2,3,7-TCDF
Chemical Name: 1,2,3,7-tetrachlorodibenzofuran
CAS Registry No: 83704-22-7
Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$
Molecular Weight: 305.978
Melting Point (°C):
167.5–168 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
438.3 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
260.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
84.4 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
122.879 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
83 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0805 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0306; 0.0805 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
4.2×10^{-6}, 1.9×10^{-4}, 5.2×10^{-3}, 8.9×10^{-2}, 1.1 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
7.08×10^{-4} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
1.41×10^{-4}, 7.08×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
$\log (P_L/\text{mmHg}) = 36.07 - 6015/(T/K) - 8.399 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
2.57 (calculated-SOFA model, Govers & Krop 1998)
1.78; 2.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.31 (calculated-SOFA model, Govers & Krop 1998)
6.04; 6.31 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
3.41 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
4.93 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.23; 4.93 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

7.07	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.10; 7.07	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2}$ = 220 min in isooctane solution, and solid phase photolysis $t_{1/2}$ = 95 h with PCDF dispersed as solid films (Buser 1988)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (4.9 – 6.0) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (1.4 – 8.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime τ = 1.9–11 d, using a 12-h average daytime OH radical concn of 1.5 × 10^6 $molecule/cm^3$ for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k_{OH}(calc) = (0.8 – 1.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated lifetime τ = 7.7–18 d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 142 L kg^{-1} d^{-1}; k_2 = 0.007 d^{-1} (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 171 L kg^{-1} d^{-1}, 220 L kg^{-1} d^{-1} (average k_1 for TCDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10^6 $molecule/cm^3$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

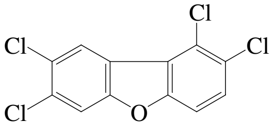
Ground water:

Sediment: degradation $t_{1/2}$ = 20–200 yr for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2}$ = 96 d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.13 1,2,7,8-Tetrachlorodibenzofuran



Common Name: 1,2,7,8-Tetrachlorodibenzofuran
Synonym:
Chemical Name: 1,2,7,8-tetrachlorodibenzofuran
CAS Registry No: 58802-20-3
Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$
Molecular Weight: 305.978
Melting Point (°C):
210–211 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
438.3 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
260.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
81.5 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
120.604 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
76 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0496 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0273; 0.0496 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.67×10^{-4} (estimated, Van den Berg et al. 1985)
1.30×10^{-4} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
2.4×10^{-6}, 1.0×10^{-4}, 2.610^{-3}, 4.2×10^{-2}, 0.49 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
3.55×10^{-4} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
$\log (P_L/\text{mmHg}) = 35.97 - 6020/(T/K) - 8.399\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
1.047×10^{-4}, 3.35×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
2.09 (calculated-SOFA model, Govers & Krop 1998)
1.70; 2.09 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.23 (shake flask-slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989)
6.41 (calculated-SOFA model, Govers & Krop 1998)
5.964 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
6.10; 6.41 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

4.97	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.22; 4.97	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

7.20	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.24; 7.20	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: sunlight induced photolysis $t_{½}$ = 220 min in isooctane solution, and solid phase photolysis half-life, $t_{½}$ = 35 h with PCDF dispersed as solid films (Buser 1988);

k = 0.014 min^{-1} with $t_{½}$ = 50 min in pure water and k = 0.0041 min^{-1} with $t_{½}$ = 170 min in 60 % acetonitrile/water solution in Corex centrifuge bottles at 300 nm photochemical reactor; k = 0.08 h^{-1} with $t_{½}$ = 8.3 h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.4–8.3) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = $(0.8–1.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 162, 130 L kg^{-1} d^{-1}; k_2 = 0.14, >1.0 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 171 L kg^{-1} d^{-1}, 220 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3}, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

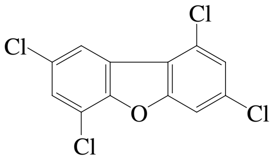
Ground water:

Sediment: degradation $t_{½}$ = 20–200 yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{½}$ = 4.9 d for PBO treated goldfish, and $t_{½}$ < 0.7 d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.14 1,3,6,8-Tetrachlorodibenzofuran



Common Name: 1,3,6,8-Tetrachlorodibenzofuran
Synonym:
Chemical Name: 1,3,6,8-tetrachlorodibenzofuran
CAS Registry No: 71998-72-6
Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$
Molecular Weight: 305.978
Melting Point (°C):
177–178 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
438.3 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
260.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
83.8 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
122.36 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
81 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.212 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0625; 0.212 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.6×10^{-6}, 1.6×10^{-4}, 4.3×10^{-3}, 7.4×10^{-2}, 0.88 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
1.17×10^{-3} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
$\log (P_L/\text{mmHg}) = 36.34 - 6020/(T/K) - 8.399 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
2.95×10^{-4}, 1.17×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.62 (calculated-SOFA model, Govers & Krop 1998)
2.04; 1.62 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.37 (shake flask/slow stirring-GC/MS, fly-ash extract, Sijm et al. 1989)
6.06 (calculated-SOFA model, Govers & Krop 1998)
5.92; 6.06 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

5.0	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.23; 5.0	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

6.71	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.76; 6.71	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (1.4–8.3) × 10^{-12} cm^3 molecule^{-1} s^{-1} for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

k_{OH}(calc) = (0.8–1.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3}, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radicals (Kwok et al. 1995).

Surface water:

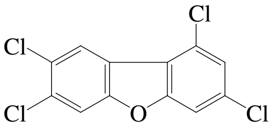
Ground water:

Sediment: degradation $t_{½}$ = 20–200 yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota:

9.1.1.15 1,3,7,8-Tetrachlorodibenzofuran



Common Name: 1,3,7,8-Tetrachlorodibenzofuran
Synonym: 1,3,7,8-TCDF
Chemical Name: 1,3,7,9-tetrachlorodibenzofuran
CAS Registry No: 57117-35-8
Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$
Molecular Weight: 306
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
260.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.116 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0463; 0.116 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):
6.03×10^{-4} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
2.00×10^{-4}, 6.03×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
3.51×10^{-5} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
$\log (P_L/\text{mmHg}) = 36.20 - 6020/(T/K) - 8.399 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.55 (calculated-SOFA model, Govers & Krop 1998)
1.91; 1.55 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)
6.20 (calculated-SOFA model, Govers & Krop 1998)
5.98; 6.20 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
3.83 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
5.01 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.23; 5.01 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:
6.90 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.95; 6.90 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (4.9 – 6.0) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (1.4 – 8.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime τ = 1.9–11 d, using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3 for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k_{OH}(calc) = (0.8 – 1.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated lifetime τ = 7.7–18 d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 164, 293 L kg^{-1} d^{-1}; k_2 < 0.1, > 1.4 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 171 L kg^{-1} d^{-1}, 220 L kg^{-1} d^{-1} (average k_1 for TCDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3, the tropospheric lifetime of a tetra-CDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

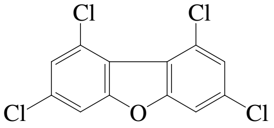
Ground water:

Sediment: degradation $t_{½}$ = 20–200 yr for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{½}$ >7 d for PBO treated goldfish and $t_{½}$ < 0.5 d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.16 1,3,7,9-Tetrachlorodibenzofuran



Common Name: 1,3,7,9-Tetrachlorodibenzofuran
Synonym: 1,3,7,9-TCDF
Chemical Name: 1,3,7,9-tetrachlorodibenzofuran
CAS Registry No: 64560-17-4
Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$
Molecular Weight: 305.978
Melting Point (°C):
206.5–207.5 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
438.3 (calculated, Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
260.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
83.3 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
121.988 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
80 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.104 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0422; 0.104 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.5×10^{-6}, 1.1×10^{-4}, 2.7×10^{-3}, 4.5×10^{-2}, 0.51 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
4.37×10^{-4} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
1.78×10^{-4}, 4.36×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
$\log (P_L/\text{mmHg}) = 36.15 - 6018/(T/K) - 8.399 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.26 (calculated-SOFA model, Govers & Krop 1998)
1.86; 1.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)
6.22 (calculated-SOFA model, Govers & Krop 1998)
6.00; 6.22 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
3.83 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
5.06 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.23; 5.06 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

6.91 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.00; 6.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

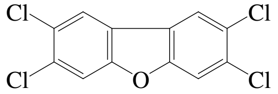
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 8.3×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)
k_{OH} = $(1.4–8.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} (Atkinson 1991)
k_{OH}(calc) = $(0.8–1.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 164, 293 L kg^{-1} d^{-1}; k_2 < 0.1, >1.4 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
k_1 = 171 L kg^{-1} d^{-1}, 220 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3}, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991);
calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).
Surface water:
Ground water:
Sediment: degradation $t_{½}$ = 20–200 yr in sediment for all homologues (Suzuki et al. 2000)
Soil:
Biota: $t_{½}$ >7 d for PBO treated gold fish and $t_{½}$ < 0.5 d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.17 2,3,7,8-Tetrachlorodibenzofuran



Common Name: 2,3,7,8-Tetrachlorodibenzofuran
Synonym: 2,3,7,8-TCDF
Chemical Name: 2,3,7,8-Tetrachlorodibenzofuran
CAS Registry No: 51207-31-9
Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$
Molecular Weight: 305.978
Melting Point (°C):
  227 (Lide 2003)
Boiling Point (°C):
  438.3 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  260.3 (calculated-Le Bas method at normal boiling point)
  199.4 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  80.3 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
  119.699 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  36.6 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  73.2 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
  0.0104 (calculated-assuming ΔS_{fus} = 56 J/mol K and mp = 227°C)
  0.00256 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  4.19×10^{-4} (22.7°C, generator column-HPLC/LSC, Friesen et al. 1990)
  3.51×10^{-3} (calculated-QSAR, Fiedler & Schramm 1990)
  4.20×10^{-4}; 5.32×10^{-4} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
  0.0413; 0.0413 (supercooled liquid S_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
  $\log [S_L/(mol/L)] = 0.655 - 1915/(T/K)$, (supercooled liquid, Passivirta et al. 1999)
  0.0243; 0.0413 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  2.0×10^{-6} (quoted, Van den Berg & Olie 1985)
  2.0×10^{-6}, 8.5×10^{-5}, 2.1×10^{-3}, 3.3×10^{-2}, 0.38 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
  1.23×10^{-4} (GC-RT correlation, supercooled liquid P_L, Eitzer & Hites 1988, 1991; quoted, Della Site 1997)
  1.13×10^{-4} (GC-RT correlation, supercooled liquid P_L, Eitzer & Hites 1989; quoted, Della Site 1997)
  2.00×10^{-4} (supercooled liquid P_L, Falconer & Bidleman 1994; quoted, Kaupp & McLachlan 1999)
  1.23×10^{-6}, 1.13×10^{-6} (calculated from reported P_L, solid vapor pressures, Della Site 1997)
  7.50×10^{-4} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)
  1.62×10^{-4}; 3.72×10^{-4} (supercooled liquid P_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
  7.39×10^{-4}; 1.89×10^{-6} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
  $\log (P_S/Pa) = 12.48 - 5425/(T/K)$ (solid, Passivirta et al. 1999)
  $\log (P_L/Pa) = 8.66 - 3513/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.678×10^{-5} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
1.718×10^{-3} (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
$\log (P_L/\text{mmHg}) = 35.91 - 6019/(T/K) - 8.399 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
8.91×10^{-5}, 3.72×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
1.50 (calculated for tetrachloro-PCDFs, Eitzer & Hites 1989)
1.70 (gas stripping-GC, 21°C, Friesen et al. 1993)
1.17; 2.69 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
$\log [H/(\text{Pa m}^3/\text{mol})] = 8.01 - 1598/(T/K)$ (Passivirta et al. 1999)
1.66; 2.69 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
5.82 (HPLC-RT correlation, Burkhard & Kuehl 1986)
6.53 (shake flask/slow stirring-GC/MS, from mixture of fly ash extract, Sijm et al. 1989)
6.19 (correlated, Ma et al. 1990)
7.10 (calculated-QSAR, Fiedler & Schramm 1990)
7.70 (calculated, Broman et al. 1991)
5.83 (HPLC-RT correlation, Jackson et al. 1993)
6.53 (recommended, Hansch et al. 1995)
6.46 (calculated-SOFA model, Govers & Krop 1998)
6.46, 6.58 (quoted, calculated-solubility log S_L and regression from lit. log K_{OW}, Passivirta et al. 1999)
6.225 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
6.13; 6.46 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
9.42 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
10.02; 9.44 (generator column-GC/ECD; calculated, Harner et al. 2000)
10.90 (7°C, GC retention time correlation, Harner et al. 2000)
$\log K_{OA} = -4.92 + 4450/(T/K)$; temp range 10–50°C (Harner et al. 2000)

Bioconcentration Factor, log BCF:
4.82 (guppy, Opperhuizen et al. 1986)
3.78, 3.39 (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988)
3.64, 3.41 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
3.82 (guppy, quoted, Opperhuizen & Sijm 1990)
4.19; 4.12 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.19; 4.33; 5.02 (guppies, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
4.93 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.23, 6.53 (fish with 5% lipid: wet weight basis, lipid weight basis, Geyer et al. 2000)
6.54, 5.75 (fish muscle log BCF_L calculated from water, sediment, Wu et al. 2001)
5.22; 4.93 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:
5.20 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
7.50 (calculated, Broman et al. 1991)
6.62 (calculated-K_{OW}, Kollig 1993)
5.18; 5.34 (sediment in lake mesocosm, Muir et al. 1992)
7.08; 7.29 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.32; 7.29 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: sunlight induced photolysis $t_{½}$ = 220 min in isooctane solution, and solid phase $t_{½}$ = 120 h with PCDF dispersed as solid films (Buser 1988);

photolytic $t_{½}$ = 9.8 h in extract of fly-ash and in tetradecane solution for native congener and $t_{½}$ = 3.0 h for ^{13}C-labelled congener (Tysklind & Rappe 1991).

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 2.3×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1987b)

k_{O3} = 1.32×10^5 L g^{-1} min^{-1} oxidative degradation rate constant for water dissolved PCDF by ozone under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987);

k_{OH}(calc) = $(2.4 – 3.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(1.4 – 8.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with calculated tropospheric lifetime τ = 1.9–11 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k_{OH}(calc) = $(0.8 – 1.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with a calculated lifetime τ = 7.7–18 d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 400 d^{-1}; k_2 = 0.062 d^{-1} (guppy, exposed to fly-ash extract, Opperhuizen et al. 1986)

k_1 = 1228, 6853 d^{-1}; k_2 = 0.28, 2.60 d^{-1} (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988)

k_1 = 56, 453 L kg^{-1} d^{-1}; k_2 < 0.1, 0.22 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 171 L kg^{-1} d^{-1}, 220 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 = 0.0058 d^{-1} with a biological $t_{½}$ = 58 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

k_1 = 603 L kg^{-1} d^{-1}; k_2 = 0.292 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994a)

k_2 = 0.0263 d^{-1} with $t_{½}$ = 26 d (newly contaminated oysters, Gardinali et al. 2004)

k_2 = 0.0194 d^{-1} with $t_{½}$ = 36 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3}, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be 7.7–18 d for the gas-phase reaction with OH radical (Kwok et al. 1995);

$t_{½}$ = 320 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{½}$ = 90 min in isooctane solution in summer sunlight (Palauschek & Scholz 1987);

suggested $t_{½}$ = 6400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{½}$ = 61 yr (Geyer et al. 2000)

degradation $t_{½}$ = 20–200 yr in sediment for all homologues (Suzuki et al. 2000)

$t_{½}$ = 550 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{½}$ = 5–50 yr in soil (Suzuki et al. 2000)

$t_{½}$ = 550 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: Elimination $t_{½}$ = 2 d from rat (Birnbaum et al. 1980; quoted, Birnbaum 1985);

$t_{½}$ = 8 d from monkey (Birnbaum et al. 1981; quoted, Birnbaum 1985);

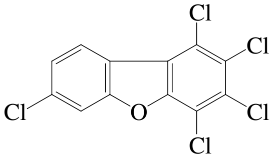
$t_{½}$ = 2–4 d from mouse (Decad et al. 1981b; quoted, Birnbaum 1985);

$t_{½}$ = 40 d from guinea pig (Decad et al. 1981a; Ioannou et al. 1983; quoted, Birnbaum 1985);

elimination half-lives: in guinea pigs, 20 d; rats, < 2 d; monkeys, 8 d; and mice, 2–4 d (quoted, Van den Berg & Olie 1985);

$t_{½}$ < 336 d in carp (Kuehl et al. 1987);
elimination $t_{½}$ = 3.0 d, 0.27 d (rainbow trout, exposed to 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988);
elimination $t_{½}$ = 0.8 d for lactating cows (Olling et al. 1991);
$t_{½}$ >7 d for PBO treated goldfish, $t_{½}$ = 3.1 d for control fish in 120-h exposure studies (Sijm et al. 1993)
elimination $t_{½}$ = 111 d from soft-shell clam (Brown 1994).
biological $t_{½}$ = 58 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)
Depuration $t_{½}$ = 26 d for newly contaminated oysters, and $t_{½}$ = 36 d for chronically contaminated oysters (Gardinali et al. 2004)

9.1.1.18 1,2,3,4,7-Pentachlorodibenzofuran



Common Name: 1,2,3,4,7-Pentachlorodibenzofuran
Synonym: 1,2,3,4,7-PCDF
Chemical Name: 1,2,3,4,7-pentachlorodibenzofuron
CAS Registry No: 83704-48-7
Molecular Formula: $C_{12}H_3Cl_5O$, $C_6Cl_4OC_6H_3Cl$
Molecular Weight: 340.418
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
281.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0179 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.00745; 0.0179 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.43×10^{-5} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
2.09×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
$\log (P_L/\text{mmHg}) = 34.22 - 6088/(T/K) - 7.865 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
1.905×10^{-5}, 1.202×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol):
2.24 (calculated-SOFA model, Govers & Krop 1998)
1.35; 2.24 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.53 (shake flask/slow stirring-GC/MS, mixture of fly-ash extract, Sijm et al. 1989)
6.89 (calculated-SOFA model, Govers & Krop 1998)
6.45; 6.89 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
4.80 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.13; 4.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:
7.89 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
8.06; 7.89 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (3.6 – 4.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (1.0 – 4.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime τ = 3.6–15 d, using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3 for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k_{OH}(calc) = (0.5 – 1.0) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated lifetime τ = 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 68 L kg^{-1} d^{-1} (goldfish after 120-h exposure: control fish, Sijm et al. 1993)

k_1 = 110 L kg^{-1} d^{-1}, 174 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 > 0.5, < 1.7 d^{-1} (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3}, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991)

calculated tropospheric lifetime to be15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995)

Surface water:

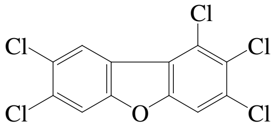
Ground water:

Sediment:

Soil:

Biota: $t_{1/2}$ < 1.4 d for PBO treated goldfish and $t_{1/2}$ < 0.4 d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.19 1,2,3,7,8-Pentachlorodibenzofuran



Common Name: 1,2,3,7,8-Pentachlorodibenzofuran
Synonym:
Chemical Name:
CAS Registry No: 57117-41-6
Molecular Formula: $C_{12}H_3Cl_5O$, $C_6HCl_3OC_6H_2Cl_2$
Molecular Weight: 340.418
Melting Point (°C):
225–227 (Rordorf 1989)
Boiling Point (°C):
464.7 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
281.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
83.6 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
128.978 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
42.4 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
85 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0108 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(\text{mol/L})] = 0.794 - 2223/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
0.0679; 0.0108 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.27×10^{-5} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
2.3×10^{-7}, 1.5×10^{-5}, 4.0×10^{-4}, 8.0×10^{-3}, 0.11 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
6.17×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
2.40×10^{-4}; 2.35×10^{-7} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/\text{Pa}) = 12.67 - 5750/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 8.23 - 3529/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
1.084×10^{-6} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
1.084×10^{-4} (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
$\log (P_L/\text{mmHg}) = 34.15 - 6081/(T/K) - 7.865 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
1.70×10^{-3}, 6.17×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol or as indicated and reported temperature dependence equations):
1.91 (calculated-SOFA model, Govers & Krop 1998)
$\log (H/(\text{Pa m}^3/\text{mol})) = 7.44 - 1306/(T/K)$ (Passivirta et al. 1999)
1.35; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

6.79	(shake flask/slow stirring-GC/MS, Sijm et al. 1989)
6.99	(calculated-SOFA model, Govers & Krop 1998)
7.07	(estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
6.47; 6.99	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.4	(7°C, GC retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log K_B:

3.38	(guppy, Opperhuizen et al. 1986)
3.84, 3.61	(gold fish: treated with metabolic inhibitor PBO, control fish, 120-h exposure, Sijm et al. 1993)
4.84	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.12; 4.84	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

7.60	(Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
8.03	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
8.11; 8.03	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution, $t_{½}$ = 10.0 h for native congener (Tysklind & Rappe 1991)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 2.5×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(1.0 - 4.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with calculated tropospheric lifetime of 3.6–15 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k_{OH}(calc) = $(0.5 - 1.0) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with a calculated lifetime of 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 98, 252 L kg^{-1} d^{-1}; k_2 < 0.1, < 0.1 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 110 L kg^{-1} d^{-1}, 174 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 = 0.0126 d^{-1} with a biological $t_{½}$ = 24 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3}, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991);
calculated room temp. tropospheric lifetime to be15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995);
suggested $t_{½}$: = 660 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{½}$ = 13200 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

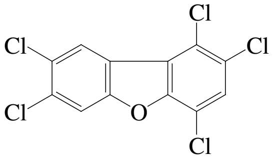
Ground water:

Sediment: $t_{½}$ = 450000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{½}$ = 450000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: elimination $t_{½}$ = 3.3–3.5 d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);
$t_{½}$ >7 d for PBO treated goldfish and $t_{½}$ >7 d for control fish in 120-h exposure studies (Sijm et al. 1993)
biological $t_{½}$ = 24 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.20 1,2,4,7,8-Pentachlorodibenzofuran



Common Name: 1,2,4,7,8-Pentachlorodibenzofuran
Synonym: 1,2,4,7,8-PeCDF
Chemical Name: 1,2,.4,7,8-pentachlorodibenzofuran
CAS Registry No: 83704-51-2
Molecular Formula: $C_{12}H_3Cl_5O$, $C_6HCl_3OC_6H_2Cl_2$
Molecular Weight: 340.418
Melting Point (°C):
236–238 (Rordorf 1989)
Boiling Point (°C):
464.7 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
281.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
85.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
128.442 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
42.4 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
89 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00179 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.00618; 0.00179 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.0×10^{-7}, 1.1×10^{-5}, 3.4×10^{-4}, 6.7×10^{-3}, 0.091 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
8.92×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
2.34×10^{-5}, 8.91×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
$\log (P_L/\text{mmHg}) = 34.28 - 6082/(T/K) - 7.865 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.62 (calculated-SOFA model, Govers & Krop 1998)
1.35; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.26 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)
6.87 (calculated-SOFA model, Govers & Krop 1998)
6.40; 6.87 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

3.02	(gold fish: treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
4.85	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.15; 4.85	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

7.86	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.96; 7.86	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 48.5 d on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (1.8 – 1,8) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (1.0 – 4.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime of 3.6–15 d, using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k_{OH}(calc) = (0.5 – 1.0) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated lifetime of 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 63, 77 L kg^{-1} d^{-1}; k_2 < 0.1, > 1.3 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 110 L kg^{-1} d^{-1}, 174 L kg^{-1} d^{-1} (average k_1 for P_5CDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3}, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991);

calculated tropospheric lifetime τ =15–29 d for the gas-phase reaction with OH radical at room temp. (Kwok et al. 1995);

suggested $t_{½}$ = 660 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: suggested $t_{½}$ = 13200 h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000)

Ground water:

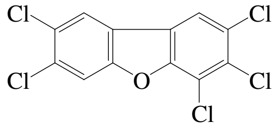
Sediment: suggested $t_{½}$ = 450000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{½}$ = 450000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: elimination $t_{½}$ = 3.3–3.5 d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);

$t_{½}$ >7 d for metabolic inhibitor PBO treated gold fish and $t_{½}$ < 1.5 d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.21 2,3,4,7,8-Pentachlorodibenzofuran



Common Name: 2,3,4,7,8-Pentachlorodibenzofuran
Synonym: 2,3,4,7,8-PCDF
Chemical Name: 2,3,4,7,8-pentachlorodibenzofuran
CAS Registry No: 57117-31-4
Molecular Formula: $C_{12}H_3Cl_5O$, $C_6H_2Cl_2OC_6HCl_3$
Molecular Weight: 340.418
Melting Point (°C):
  196–196.5 (Kuroki et al. 1984, Rordorf 1989)
Boiling Point (°C):
  464.7 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  281.2 (calculated-Le Bas method at normal boiling point)
  212.3 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  85.6 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
  130.43 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  42.4 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  90 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
  0.0208 (calculated-assuming ΔS_{fus} = 56 J/mol K and mp = 196.5°C)
  0.00196 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  0.000515 (calculated-QSAR, Fiedler & Schramm 1990)
  0.000236 (22.7°C, generator column-GC/MS, Friesen et al. 1990)
  0.00015 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
  0.0115; 7.11×10^{-3} (supercooled liquid S_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
  $\log [S_L/(\text{mol/L})] = 1.076 - 2218/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
  0.00481; 0.00711 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  2.17×10^{-5} (supercooled liquid P_L-GC-RT correlation, Eitzer & Hites 1988, 1991)
  2.43×10^{-5} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
  3.5×10^{-7}, 2.1×10^{-5}, 6.7×10^{-4}, 1.4×10^{-2}, 0.19 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
  1.74×10^{-5} (supercooled liquid P_L, Falconer & Bidleman 1994; quoted, Kaupp & McLachlan 1999)
  1.53×10^{-4} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)
  1.95×10^{-5}; 5.50×10^{-5} (supercooled liquid P_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
  1.91×10^{-4}; 3.74×10^{-7} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
  $\log (P_S/\text{Pa}) = 12.62 - 5677/(T/K)$ (solid, Passivirta et al. 1999)
  $\log (P_L/\text{Pa}) = 7.90 - 3462/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

6.53×10^{-6} (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)
3.20×10^{-4} (supercooled liquid P_L, calculated from P_S assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)
$\log (P_L/\text{mmHg}) = 33.99 - 6084/(T/K) - 7.865\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
1.15×10^{-5}, 5.50×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa m^3/mol or as indicated and reported temperature dependence equations):
0.505 (calculated-P/C with selected values)
0.575; 2.57 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
$\log (H/(\text{Pa m}^3/\text{mol})) = 6.82 - 1244/(T/K)$ (Passivirta et al. 1999)
1.29; 2.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.92 (shake flask/slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989)
7.82 (calculated-QSAR, Fiedler & Schramm 1990)
7.60 (calculated, Broman et al. 1991)
6.92 (recommended, Hansch et al. 1995)
7.11 (calculated-SOFA model, Govers & Krop 1998)
7.11, 6.90 (quoted, calculated-solubility log S_L and regression from lit. log K_{OW}, Passivirta et al. 1999)
6.757 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
6.56; 7.11 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.09 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
11.52 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF:
3.70 (guppy, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990)
5.14; 4.92 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
5.14; 5.15; 5.38 (guppies, 21-d exposure, lipid weight basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
5.14; 4.79 (lipid wt basis, quoted exptl.; quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
5.62; 5.92, 6.92 (fish 5% lipid: wet wt basis; fish 10% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
6.42, 5.88 (fish muscle log BCF_L calculated from water, sediment, Wu et al. 2001)
5.08; 4.79 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Bioaccumulation Factor, BAF:
1.44, 1.33 (rainbow trout, concn in food: 0.82, 9.01 ng/g, Muir et al. 1990)

Sorption Partition Coefficient, log K_{OC}:
5.59 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
7.40 (calculated, Broman et al. 1991)
6.60, 6.92 (calculated-K_{OW}, Kollig 1993)
8.20 (calculated-SOFA model, sediment/water, Govers & Krop 1998)
8.30; 8.20 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis: photolytic degradation $t_{1/2}$ = 3.5 h of PCDD in extract of fly-ash in tetradecane solution for native congener and $t_{1/2}$ = 3.1 h for ^{13}C-labelled congener (Tysklind & Rappe 1991)
$t_{1/2}$ = 55.0 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)
Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (1.7 –1.8) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = (1.0 – 4.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime τ = 3.6–15 d, using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k_{OH}(calc) = (0.5 – 1.0) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated lifetime τ = 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.0027 d^{-1} (carp, calculated from data reported by Kuehl et al. 1987, Sijm et al. 1990)

k_1 = 400 mL g^{-1} d^{-1}; k_2 = 0.079 d^{-1} (guppy, Opperhuizen et al. 1986)

k_2 = 0.0064 d^{-1} (liver of female rat, Van den Berg et al. 1989)

k_2 = –2.1 × 10^{-2}, 1.5 × 10^{-2} d^{-1} (rainbow trout, 2 to 21 d exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1990)

k_2 = 10.1 × 10^{-3} d^{-1} and k_2 = 8.10 × 10^{-3} d^{-1}; k_2 = 12.6 × 10^{-3} d^{-1} and k_2 = 11.4 × 10^{-3} d^{-1} (rainbow trout, 0–140 d and 0–180 d exposure at 0.82 ng/g PCDF concn.; 0–140 d and 0–180 d exposure at 9.01 ng/g PCDF concn., Muir et al. 1990)

k_1 = 105, 561 L kg^{-1} d^{-1}; k_2 = 0.11, < 0.1 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 110 L kg^{-1} d^{-1}, 174 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 = 0.0081 d^{-1} with a biological $t_{1/2}$ = 36 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

k_1 = 1012 L kg^{-1} d^{-1}; k_2 = 0.044 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3}, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995);

$t_{1/2}$ = 660 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolytic $t_{1/2}$ = 3.5 h in the extract from fly-ash in tetradecane solution, for native congener and $t_{1/2}$ = 3.1 h for ^{13}C labelled congener (Tysklind & Rappe 1991)

$t_{1/2}$ = 13200 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{1/2}$ = 60 yr (Geyer et al. 2000)

degradation $t_{1/2}$ = 20–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2}$ = 550 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2}$ = 5–50 yr (estimated, Suzuki et al. 2000);

$t_{1/2}$ = 550 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2}$ = 108 d in the liver of female rats (Van den Berg et al. 1989);

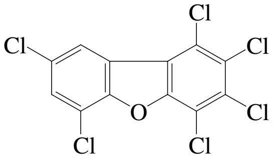
$t_{1/2}$ = 69 d in rainbow trout at the 0.82 ng/g exposure concentration from 0–140 d data, $t_{1/2}$ = 61 d at 9.0 ng/g exposure concentration from 0–180 d data; $t_{1/2}$ = 65 d in whole body rainbow trout with 31-d dietary exposure (Muir et al. 1990);

elimination $t_{1/2}$ = 48.5 d for lactating cows (Olling et al. 1991);

$t_{1/2}$ = 6.1 d for PBO treated goldfish and $t_{1/2}$ > 7 d for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2}$ = 49 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.22 1,2,3,4,6,8-Hexachlorodibenzofuran



Common Name: 1,2,3,4,6,8-Hexachlorodibenzofuran
Synonym: 1,2,3,4,6,8-HxCDF
Chemical Name: 1,2,3,4,6,8-Hexachlorodibenzofuran
CAS Registry No: 69698-60-8
Molecular Formula: $C_{12}H_2Cl_6O$, $C_6H_2Cl_2OC_6Cl_4$
Molecular Weight: 374.863
Melting Point (°C):
  233.5–234 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
  487.7 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  302.1 (calculated-Le Bas method at normal boiling point)
  225.2 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  86 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
  137.049 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  48.1 (Rordorf 1989; quod, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  95 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F :
  0.000332 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
  6.08×10^{-3} (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
  $\log [S_L/(mol/L)] = 0.839 - 2520/(T/K)$, (supercooled liquid, Passivirta et al. 1999)
  2.48×10^{-3}, 5.08×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  2.9×10^{-8}, 2.1×10^{-6}, 8.1×10^{-5}, 1.9×10^{-3}, 0.031 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
  7.67×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
  1.74×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
  9.39×10^{-5}; 4.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
  $\log (P_S/Pa) = 12.84 - 6057/(T/K)$ (solid, Passivirta et al. 1999)
  $\log (P_L/Pa) = 7.88 - 3540/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
  5.13×10^{-6}, 1.74×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
  $\log (P_L/mmHg) = 32.06 - 6015/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C):
  1.023 (calculated-SOFA model, Govers & Krop 1998)
  $\log (H/(Pa\ m^3/mol)) = 7.04 - 1020/(T/K)$ (Passivirta et al. 1999)
  1.26; 1.012 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.31 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.58 (calculated-solubility log S_L and regression from lit. log K_{OW}s, Passivirta et al. 1999)
6.78; 7.31 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

4.66 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
4.96; 4.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

8.47 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
8.72; 8.47 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

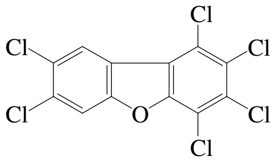
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: $t_{½}$ = 59.8 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 0.74×10^{-12} cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)
k_{OH} = $(0.7 - 2.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 168 L kg^{-1} d^{-1}; k_2 < 0.1 d^{-1} (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)
k_1 = 110 L kg^{-1} d^{-1}, 174 L kg^{-1} d^{-1} (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
suggested $t_{½}$ = 1400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: suggested $t_{½}$ = 28 000 h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: degradation $t_{½}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000);
suggested $t_{½}$ = 450 000 h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).
Soil: degradation $t_{½}$ = 5–50 yr (estimated, Suzuki et al. 2000);
suggested $t_{½}$ = 450 000 h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).
Biota: $t_{½}$ >7 d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993)

9.1.1.23 1,2,3,4,7,8-Hexachlorodibenzofuran



Common Name: 1,2,3,4,7,8-Hexachlorodibenzofuran
Synonym: 1,2,3,4,7,8-HxCDF
Chemical Name: 1,2,3,4,7,8-Hexachlorodibenzofuran
CAS Registry No: 70658-26-9
Molecular Formula: $C_{12}H_2Cl_6O$, $C_6H_2Cl_2OC_6Cl_4$
Molecular Weight: 374.863
Melting Point (°C):
225.5–226.5 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
487.7 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
302.1 (calculated-Le Bas method at normal boiling point)
225.2 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
86.5 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
137.397 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
48.1 (Rordorf 1989; quod, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
96 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F :
0.0107 (calculated-assuming ΔS_{fus} = 56 J/mol K and mp = 226°C)
0.000402 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
8.25×10^{-6} (22.7°C, generator column-GC/MS, Friesen et al. 1990)
7.30×10^{-6} (computed-expert system SPARC, Kollig 1995)
8.2×10^{-6}, 1.13×10^{-6} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
8.01×10^{-4}; 2.65×10^{-3} (supercooled liquid S_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(mol/L)] = 0.913 - 2516/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
1.64×10^{-3}, 2.65×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
8.093×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988; quoted, Della Site 1997)
3.2×10^{-8}, 2.4×10^{-6}, 9.3×10^{-5}, 2.2×10^{-3}, 0.036 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
7.85×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989; quoted, Della Site 1997)
8.90×10^{-8} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
3.09×10^{-6} (supercooled liquid P_L, Falconer & Bidleman 1994;)
8.67×10^{-8} (computed-expert system SPARC, Kollig 1995)
8.41×10^{-8}, 3.68×10^{-8} (P_S solid vapor pressure calculated from reported P_L, Della Site 1997)

6.05×10^{-5} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)
5.62×10^{-6}; 1.38×10^{-5} (supercooled liquid P_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
2.87×10^{-8}; 7.13×10^{-5} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/\text{Pa}) = 12.85 - 6077/(T/\text{K})$ (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 7.81 - 3564/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)
$\log (P_L/\text{mmHg}) = 32.14 - 6106/(T/\text{K}) - 7.332 \cdot \log (T/\text{K})$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
3.24×10^{-6}, 1.38×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
1.454 (calculated-P/C with selected values)
4.26 (computed-expert system SPARC, Kollig 1995)
2.63; 1.91 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
$\log [H/(\text{Pa m}^3/\text{mol})] = 6.90 - 1048/(T/\text{K})$ (Passivirta et al. 1999)
1.26; 1.905 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
7.70 (calculated, Broman et al. 1991)
7.86 (computed-expert system SPARC, Kollig 1995)
7.53 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.54 (calculated-solubility log S_L and regression from lit. log K_{OW}, Passivirta et al. 1999)
7.184 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
6.92; 7.53 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.64 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
11.98 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF:
4.91; 4.40 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.91; 4.99; 5.04 (guppies, 21-d exposure, lipid weight basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
4.57 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.90, 5.26 (fish muscle log BCF_L calculated from water, sediment, Wu et al. 2001)
4.88; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:
7.40 (calculated, Broman et al. 1991)
7.54 (computed-expert system SPARC, Kollig 1995)
8.83; 8.80 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
8.95; 8.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis: photolytic $t_{½}$ =5.5 h of the PCDD in extract of fly ash in tetradecane solution for native congener (Tysklind & Rappe 1991).
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{O3}(aq.) = 7.28×10^4 L·g^{-1}·min^{-1}, oxidative degradation rate constant of water dissolved PDCF by ozone under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH} = (0.7–2.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for a hexa-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 5.9–22 d using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule cm^{-3} (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 100, 439 L kg^{-1} d^{-1}; k_2 = 0.31, < 0.1 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 110 L kg^{-1} d^{-1}, 174 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 = 0.0126 d^{-1} with a biological $t_{1/2}$ = 24 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

k_1 = 879 L kg^{-1} d^{-1}; k_2 = 0.087 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2}$ = 1400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2}$ = 28 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2}$ = 600 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2}$ = 5–50 yr (estimated, Suzuki et al. 2000);

$t_{1/2}$ = 600 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

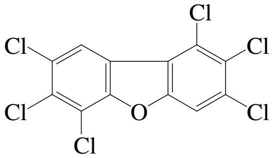
Biota: $t_{1/2}$ ~ 336 d in carp (Kuehl et al. 1987);

elimination $t_{1/2}$ = 48.5 d from lactating cows (Olling et al. 1991);

$t_{1/2}$ = 2.2 d for PBO treated goldfish and $t_{1/2}$ >7 d for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2}$ = 24 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.24 1,2,3,6,7,8-Hexachlorodibenzofuran



Common Name: 1,2,3,6,7,8-Hexachlorodibenzofuran
Synonym:
Chemical Name: 1,2,3,6,7,8-hexachlorodibenzofuran
CAS Registry No: 57117-44-9
Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$
Molecular Weight: 374.863
Melting Point (°C):
 232–234 (Rordorf 1989)
Boiling Point (°C):
 487.7 (calculated, Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
 302.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 86.1 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
 137.083 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 48.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 95 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
 0.000358 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
 0.00226 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
 $\log [S_L/(\text{mol/L})] = 0.125 - 2515/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 1.56×10^{-3}, 2.26×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 7.33×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
 2.9×10^{-8}, 2.1×10^{-6}, 8.2×10^{-5}, 2.0×10^{-3}, 0.031 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
 1.20×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
 6.91×10^{-5}; 2.47×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 12.87 - 6101/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 7.91 - 3954/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P_L/\text{mmHg}) = 32.12 - 6108/(T/K) - 7.332\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 3.09×10^{-6}, 1.20×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations:
 1.91 (calculated-SOFA model, Govers & Krop 1998)
 $\log (H/(\text{Pa m}^3/\text{mol})) = 7.79 - 1439/(T/K)$, (Passivirta et al. 1999)
 1.26; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.60 (calculated, Broman et al. 1991)
7.57 (calculated-SOFA model, Govers & Krop 1998)
7.96 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
7.196 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
6.93; 7.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.0 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log K_B:

4.95; 4.49 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.95, 5.15; 5.24 (guppies, 21-d exposure, lipid weight basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
4.58 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.51 (fish muscle log BCF_L calculated from water, Wu et al. 2001)
4.87; 4.58 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

7.40 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
8.85 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
8.97; 8.85 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

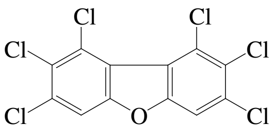
Volatilization:
Photolysis: photolytic $t_{½}$ = 5.9 h in extract of fly-ash and in tetradecane solution for native congener (Tysklind & Rappe 1991);
$t_{½}$ = 74.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(1.3 – 1.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)
k_{OH} = $(0.7 – 2.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 103, 460 L kg^{-1} d^{-1}; k_2 = 0.26, < 0.1 d^{-1} (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
k_1 = 110 L kg^{-1} d^{-1}, 174 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
k_2 = 0.0138 d^{-1} with a biological $t_{½}$ = 22 d (blue mussel, 99-d exposure, Hektoen et al. 1994)
k_1 = 1310 L kg^{-1} d^{-1}; k_2 = 0.078 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
$t_{½}$ = 1400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Surface water: $t_{½}$ = 28000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Ground water:

Sediment: $t_{1/2}$ = 700000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{1/2}$ = 700000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Biota: elimination $t_{1/2}$ = 73–156 d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);
$t_{1/2}$ = 2.7 d for PBO treated goldfish and $t_{1/2}$ >7 d for control fish in 120-h exposure studies (Sijm et al. 1993)
biological $t_{1/2}$ = 22 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994).

9.1.1.25 1,2,3,7,8,9-Hexachlorodibenzofuran



Common Name: 1,2,3,7,8,9-Hexachlorodibenzofuran
Synonym: 1,2,3,7,8,9-HxCDF
Chemical Name: 1,2,3,7,8,9-hexachlorodibenzofuran
CAS Registry No: 72918-21-9
Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$
Molecular Weight: 374.863
Melting Point (°C):
  246–249 (Rordorf 1989)
  230 (calculated, Passivirta et al. 1999)
Boiling Point (°C):
  487.7 (calculated, Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
  302.1 (calculated-Le Bas method at normal boiling point)
  225.2 (Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
  96 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.00036 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  0.000859 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
  $\log [S_L/(mol/L)] = 0.892 - 2526/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
  1.06×10^{-3}, 8.59×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  4.99×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)
  4.31×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
  3.88×10^{-5} (corrected, supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)
  2.24×10^{-6} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
  4.01×10^{-5}; 1.44×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
  $\log (P_S/Pa) = 12.91 - 6185/(T/K)$ (solid, Passivirta et al. 1999)
  $\log (P_L/Pa) = 7.90 - 3625/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
  $\log (P_L/mmHg) = 31.92 - 6114/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
  2.09×10^{-6}, 2.24×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C or as indicated and reported temperature dependence equations):
  0.955 (calculated-SOFA model, Govers & Krop 1998)
  $\log [H/(Pa\ m^3/mol)] = 7.01 - 1136/(T/K)$ (Passivirta et al. 1999)
  1.29; 0.955 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
  7.00 (calculated, Broman et al. 1991)
  7.76 (calculated-SOFA model, Govers & Krop 1998)

7.57	(estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
7.125	(calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.07; 7.76	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.17	(7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log K_B:

4.71	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.04	(fish muscle log BCF_L calculated from water, Wu et al. 2001)
4.77; 4.71	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

9.08	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
9.19; 9.08	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution: $t_{1/2}$ = 2.2 h for native congener and $t_{1/2}$ = 3.6 h for ^{13}C-labelled congener (Tysklind & Rappe 1991);

$t_{1/2}$ = 78.8 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(1.3 - 1.8) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(0.7 - 2.6) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.01651 d^{-1} with a biological $t_{1/2}$ = 18 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

k_1 = 1101 L kg^{-1} d^{-1}; k_2 = 0.103 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2}$ = 1400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2}$ = 28000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

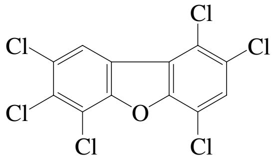
Ground water:

Sediment: $t_{1/2}$ = 500000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2}$ = 500000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: biological $t_{1/2}$ = 18 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.26 1,2,4,6,7,8-Hexachlorodibenzofuran



Common Name: 1,2,4,6,7,8-Hexachlorodibenzofuran
Synonym: 1,2,4,6,7,8-HxCDF
Chemical Name: 1,2,4,6,7,8-hexachlorodibenzofuran
CAS Registry No: 67562-40-7
Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$
Molecular Weight: 374.863
Melting Point (°C):
221–222 (Kuroki et al. 1986; Rordorf 1989; Passivirta et al. 1999)
Boiling Point (°C):
487.7 (calculated, Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
302.1 (calculated-Le Bas method at normal boiling point)
225.2 (Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
86.8 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
137.593 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
48.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
97 (Rordorf 1989; Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.000483 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
0.00451 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(\text{mol/L})] = 0.944 - 2512/(T/K)$, (supercooled liquid, Passivirta et al. 1999)
2.26×10^{-3}, 4.51×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.5×10^{-8}, 2.6×10^{-6}, 1.0×10^{-4}, 2.4×10^{-3}, 0.040 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
1.35×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
9.39×10^{-5}; 4.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/\text{Pa}) = 12.81 - 6006/(T/K)$, (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 7.74 - 3497/(T/K)$, (supercooled liquid, Passivirta et al. 1999)
4.47×10^{-6}, 2.35×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
$\log (P_L/\text{mmHg}) = 32.31 - 6108/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
1.072 (calculated-SOFA model, Govers & Krop 1998)
$\log [H/(\text{Pa m}^3/\text{mol})] = 6.80 - 985/(T/K)$, (Passivirta et al. 1999)
1.26; 1.072 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.38	(calculated-SOFA model, Govers & Krop 1998)
7.51	(estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
6.83; 7.38	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

4.66	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
4.94; 4.66	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

8.58	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
8.78; 8.58	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2}$ = 58.2 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 0.74×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(0.7 - 2.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 345, 293 L kg^{-1} d^{-1}; k_2 < 0.10, > 2.4 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 170 L kg^{-1} d^{-1}, 369 L kg^{-1} d^{-1} (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_1 = 1101 L kg^{-1} d^{-1}; k_2 = 0.103 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

suggested $t_{1/2}$ = 1400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: suggested $t_{1/2}$ = 28000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

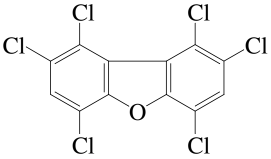
Ground water:

Sediment: suggested $t_{1/2}$ = 500000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{1/2}$ = 500000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: $t_{1/2}$ >7 d for PBO treated goldfish and $t_{1/2}$ < 0.3 d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.27 1,2,4,6,8,9-Hexachlorodibenzofuran



Common Name: 1,2,4,6,8,9-Hexachlorodibenzofuran
Synonym: 1,2,3,4,8,9-HxCDF
Chemical Name: 1,2,4,6,8,9-hexachlorodibenzofuran
CAS Registry No: 69698-59-5
Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$
Molecular Weight: 374.863
Melting Point (°C):
246–248 (Kuroki et al. 1984; Passivirta et al. 1999)
Boiling Point (°C):
487.7 (Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
302.1 (calculated-Le Bas method at normal boiling point)
225.2 (Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
85.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
136.462 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
48.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
93 (Rordorf 1989; Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.000245 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
0.00305 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(mol/L)] = 0.892 - 2526/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
1.92×10^{-3}, 3.05×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.4×10^{-8}, 1.7×10^{-6}, 6.4×10^{-5}, 1.5×10^{-3}, 0.024 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
9.22×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
3.55×10^{-6} supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
7.96×10^{-5}; 1.95×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 12.89 - 6137/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 9.08 - 3629/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
3.89×10^{-6}, 3.55×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
$\log (P_L/mmHg) = 32.22 - 6105/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
0.417 (calculated-SOFA model, Govers & Krop 1998)
$\log [H/(Pa\ m^3/mol)] = 7.40 - 1117/(T/K)$ (Passivirta et al. 1999)
1.26; 0.417 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.43	(calculated-SOFA model, Govers & Krop 1998)
7.65	(estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
6.87; 7.43	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

4.84	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
4.91; 4.84	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

8.58	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
8.86; 8.58	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 82.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 0.74×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(0.7 - 2.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 170 L kg^{-1} d^{-1}, 369 L kg^{-1} d^{-1} (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 > 2.0$ d^{-1} (120-h exposure: metabolic inhibitor PBO-treated goldfish, Sijm et al. 1993)

k_1 = 1101 L kg^{-1} d^{-1}; k_2 = 0.103 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{½}$ = 1400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{½}$ = 28000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

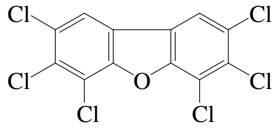
Ground water:

Sediment: $t_{½}$ = 150000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{½}$ = 150000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: $t_{½} < 0.3$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.28 2,3,4,6,7,8-Hexachlorodibenzofuran



Common Name: 2,3,4,6,7,8-Hexachlorodibenzofuran
Synonym: 2,3,4,6,7,8-HCDF
Chemical Name: 2,3,4,6,7,8-hexachlorodibenzofuran
CAS Registry No: 60851-34-5
Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$
Molecular Weight: 374.863
Melting Point (°C):
 239–240 (Rordorf 1989)
Boiling Point (°C):
 487.7 (calculated, Rordorf 1989)
Density (g/cm^3):
Molar Volume (cm^3/mol):
 302.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 85.7 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
 136.794 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 48.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 94 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
 0.000276 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
 0.00156 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
 $\log [S_L/(\text{mol/L})] = 0.787 - 2527/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 1.24×10^{-3}, 1.56×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
 4.99×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)
 5.82×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
 3.88×10^{-5} (corrected, supercooled liquid P_L, in Eitzer & Hites 1988, Eitzer & Hites 1998)
 2.6×10^{-8}, 1.9×10^{-6}, 7.3×10^{-5}, 1.7×10^{-3}, 0.028 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
 7.59×10^{-6} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
 5.54×10^{-5}; 1.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 12.91 - 6175/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 8.00 - 3651/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P_L/\text{mmHg}) = 31.99 - 6108/(T/K) - 7.332\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 2.45×10^{-6}, 7.59×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m^3/mol or as indicated and reported temperature dependence equations):
 1.78 (calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 7.21 - 1124/(T/K)$ (Passivirta et al. 1999)
 1.26; 1.78 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.0	(calculated, Broman et al. 1991)
7.65	(calculated-SOFA model, Govers & Krop 1998)
7.62	(estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
6.937	(calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.01; 7.65	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.10	(7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log K_B:

4.88	(goldfish, 120-h exposure studies, Sijm et al. 1993)
4.99; 4.94; 5.02	(guppies, 21-d exposure, lipid weight basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
4.59	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.51	(fish muscle log BCF_L calculated from water, Wu et al. 2001)
4.81; 4.59	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

6.80	(Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
8.96	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
9.10; 8.96	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution: $t_{½}$ = 2.8 h for native congener (Tysklind & Rappe 1991);

$t_{½}$ = 70.7 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 0.74×10^{-12} cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 267 L kg^{-1} d^{-1}; $k_2 < 0.1$ d^{-1} (goldfish after 120-h exposure: control fish, Sijm et al. 1993)

k_2 = 0.36 (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 110 L kg^{-1} d^{-1}, 174 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 = 0.0119 d^{-1} with a biological $t_{½}$ = 25 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{½}$ = 1400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{½}$ = 28000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Ground water:

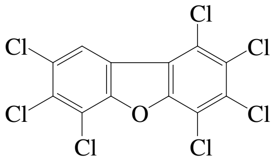
Sediment: $t_{½}$ = 500000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Soil: $t_{½}$ = 500000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: $t_{½}$ = 1.9 d for PBO treated goldfish and $t_{½}$ >7 d for control fish in 120-h exposure studies (Sijm et al. 1993).

biological $t_{½}$ = 25 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.29 1,2,3,4,6,7,8-Heptachlorodibenzofuran



Common Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran
Synonym: 1,2,3,4,6,7,8-HCDF
Chemical Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran
CAS Registry No: 67562-39-4
Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$
Molecular Weight: 409.308
Melting Point (°C):
236–237 (Kuroki et al. 1984; Rordorf 1989; Della Site 1997)
Boiling Point (°C):
507.2 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
323.0 (calculated-Le Bas method at normal boiling point)
238.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
87.8 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
144.642 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
53.9 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
106 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.000122 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
1.35×10^{-6} (22.7°C, generator column-GC/MS, Friesen et al. 1990)
1.08×10^{-5} (calculated-QSAR, Fiedler & Schramm 1990)
9.50×10^{-7} (computed-expert system SPARC, Kollig 1995)
1.26×10^{-7} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
1.63×10^{-4}; $7\ 11 \times 10^{-4}$ (supercooled liquid S_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(mol/L)] = 0.917 - 2812/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
4.92×10^{-4}, 7.11×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.24×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991; quoted, Della Site 1997)
1.93×10^{-6} (supercooled liquid P_L GC-RT correlation, Eitzer & Hites 1989; quoted, Della Site 1997)
4.7×10^{-9}, 4.3×10^{-7}, 2.0×10^{-5}, 5.8×10^{-4}, 1.1×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
5.10×10^{-8} (gas saturation method, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
8.70×10^{-9} (computed-expert system SPARC, Kollig 1995)
1.83×10^{-8}, 1.58×10^{-8} (P_S solid vapor pressure calculated from reported P_L, Della Site 1997)
1.84×10^{-5} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)
1.4×10^{-6}; 2.51×10^{-6} (supercooled liquid P_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
5.54×10^{-5}; 6.76×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

log (P_S/Pa) = 12.98 – 6302/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 7.45 – 3486/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P_L/mmHg) = 30.03 – 6090/(T/K) – 6.798·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
9.33×10^{-7}, 2.51×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa m^3/mol at 25°C):

3.80	(computed-expert system SPARC, Kollig 1995)
3.47; 1.41	(quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa m^3/mol)] = 6.53 – 674/(T/K) (Passivirta et al. 1999)	
1.41; 1.41	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.92	(shake flask/slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989a)
9.25	(calculated-QSAR, Friedler & Schramm 1990)
7.90	(quoted, Loonen et al. 1991)
8.10	(calculated, Broman et al. 1991)
7.92	(recommended, Hansch et al. 1995)
8.52	(computed-expert system SPARC, Kollig 1995)
8.01	(calculated-SOFA model, Govers & Krop 1998)
8.07	(calculated-solubility log S_L and regression from lit. log K_{OW}, Passivirta et al. 1999)
7.477	(calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.37; 8.00	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.06	(7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF:

4.46; 4.08	(guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.46; 4.60; 4.63	(guppy, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
4.46; 4.26	(lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
6.62; 6.92	(wet wt basis, fish 5% lipid, 10% lipid, Geyer et al. 2000)
5.89, 6.03	(fish muscle log BCF_L calculated from water, sediment, Wu et al. 2001)
4.51; 4.26	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

6.37	(organic carbon, calculated-QSAR, Friedler & Schramm 1990)
6.00	(organic carbon, calculated, Broman et al. 1991)
7.90	(calculated, Broman et al. 1991)
8.20	(computed-K_{OW}, Kollig 1995)
9.07; 9.48	(sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
9.64; 9.48	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolytic degradation $t_{½}$ = 9.8 h with extract of fly-ash and in tetradecane solution for native congener and $t_{½}$ = 3.7 h for ^{13}C-labelled congener (Tysklind & Rappe 1991).
$t_{½}$ = 84.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{O3}(aq.) = 1.08×10^5 L g^{-1} min^{-1}, oxidative degradation rate constant of water dissolved PCDF by ozone under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = 0.53×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(0.5 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime τ =17–31 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 42, 61 L kg^{-1} d^{-1}; k_2 = 0.43, 0.1 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 42 L kg^{-1} d^{-1}, 61 L kg^{-1} d^{-1} (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

k_2 = 0.0084 d^{-1} with a biological $t_{½}$ = 36 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

k_1 = 524 L kg^{-1} d^{-1}; k_2 = 0.127 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF with OH radicals to be 17–31 d (Atkinson 1991);

$t_{½}$ = 3200 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{½}$ = 64 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{½}$ = 36 yr (Geyer et al. 2000)

degradation $t_{½}$ = 2–200 yr for all homologues (estimated, Suzuki et al. 2000);

$t_{½}$ = 350 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{½}$ = 5–50 yr (estimated, Suzuki et al. 2000);

$t_{½}$ = 350 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

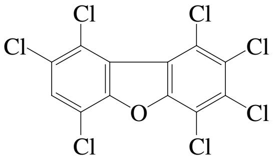
Biota: depuration $t_{½}$ > 336 d for carp in Lake Superior water (Kuehl et al. 1987);

elimination $t_{½}$ = 33.9 d from lactating cow (Olling et al. 1991);

$t_{½}$ = 1.6 d for PBO treated goldfish and $t_{½}$ = 6.8 d for control fish in 120-h exposure studies (Sijm et al. 1993).

biological $t_{½}$ = 37 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.30 1,2,3,4,6,8,9-Heptachlorodibenzofuran



Common Name: 1,2,3,4,6,8,9-Heptachlorodibenzofuran
Synonym: 1,2,3,4,6,8,9-HpCDF
Chemical Name: 1,2,3,4,6,8,9-Heptachlorodibenzofuran
CAS Registry No: 69698-58-4
Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$
Molecular Weight: 409.308
Melting Point (°C):
211–212 (Kuroki et al. 1984; Rordorf 1989; Della Site 1997)
Boiling Point (°C):
507.2 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
323.0 (calculated-Le Bas method)
238.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
89.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
145.64 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
53.9 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
111 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.00021 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
5.65×10^{-4} (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(mol/L)] = 1.200 - 2861/(T/K)$, (supercooled liquid, Passivirta et al. 1999)
4.19×10^{-4}, 5.65×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
7.7×10^{-9}, 7.2×10^{-7}, 3.6×10^{-5}, 1.0×10^{-3}, 2.0×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
7.24×10^{-7} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
1.55×10^{-5}; 3.57×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 13.03 - 6394/(T/K)$, (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 7.23 - 3581/(T/K)$, (supercooled liquid, Passivirta et al. 1999)
8.13×10^{-7}, 7.24×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
$\log (P_L/mmHg) = 29.94 - 6089/(T/K) - 6.798 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
5.13 (calculated-SOFA model, Govers & Krop 1998)
$\log [H/(Pa\ m^3/mol)] = 6.03 - 756/(T/K)$, (Passivirta et al. 1999)
1.45; 5.13 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

8.02	(calculated-SOFA model, Govers & Krop 1998)
7.91	(calculated-solubility log S_L and regression from lit. log K_{OW}, Passivirta et al. 1999)
7.43; 8.02	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

4.42	(lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
4.46; 4.42	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

9.45	(sediment/water, calculated-SOFA model, Govers & Krop 1998)
9.72; 9.45	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 85.6 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 0.53×10^{-12} cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)

$k_{OH} = (0.5 – 0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with calculated tropospheric lifetime of 17–31 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm³ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 42 L kg⁻¹ d⁻¹, 61 L kg⁻¹ d⁻¹ (average k_1 for H_7CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF with OH radical to be 17–31 d (Atkinson 1991);

suggested $t_{½}$ = 3200 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_{½}$ = 64 000 h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{½}$ = 2–200 yr for all homologues (estimated, Suzuki et al. 2000);

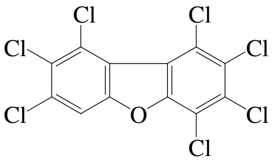
suggested $t_{½}$ = 350 000 h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Soil: degradation $t_{½}$ = 5–50 yr (estimated, Suzuki et al. 2000);

suggested $t_{½}$ = 350 000 h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Biota:

9.1.1.31 1,2,3,4,7,8,9-Heptachlorodibenzofuran



Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran
Synonym: 1,2,3,4,7,8,9-HCDF
Chemical Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran
CAS Registry No: 55673-89-7
Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$
Molecular Weight: 409.308
Melting Point (°C):
221–223 (Kuroki et al. 1984)
Boiling Point (°C):
507.2 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
323.0 (calculated-Le Bas method at normal boiling point)
248.1 (Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
88.6 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
145.221 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
53.9 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
109 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.000179 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
1.30×10^{-6} (computed-expert system SPARC, Kollig 1995)
2.58×10^{-4} (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(\text{mol/L})] = 1.100 - 2819/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
2.83×10^{-4}, 2.58×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.2×10^{-9}, 5.8×10^{-7}, 2.8×10^{-5}, 8.0×10^{-4}, 1.5×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1987, 1989)
1.305×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)
1.011×10^{-6} (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
1.27×10^{-9} (computed-expert system SPARC, Kollig 1995)
1.48×10^{-8}, 1.14×10^{-8} (solid vapor pressures calculated from reported P_L, Della Site 1997)
6.61×10^{-7} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
7.87×10^{-6}; 1.41×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/\text{Pa}) = 13.12 - 6547/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 7.23 - 3581/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
$\log (P_L/\text{mmHg}) = 29.69 - 6089/(T/K) - 6.798\cdot\log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
5.75×10^{-7}, 6.60×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa m^3/mol or as indicated and reported temperature dependence equations):

3.85	(computed-expert system SPARC, Kollig 1995)
1.0	(calculated-SOFA model, Govers & Krop 1998)

log [H/(Pa m^3/mol)] = 6.32 – 912/(T/K) (Passivirta et al. 1999)

1.58; 1.0	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

6.90	(calculated, Broman et al. 1991)
8.50	(computed-expert system SPARC, Kollig 1995)
8.23	(calculated-SOFA model, Govers & Krop 1998)
7.99	(calculated-solubility log S_L and regression from lit. log K_{OW}, Passivirta et al. 1999)
7.616	(calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.60; 8.23	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA}at 25 °C or as indicated:

12.34	(7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF:

4.32	(calculated-SOFA model, Govers & Krop 1998)
5.59	(fish muscle log BCF_L calculated from water, Wu et al. 2001)
4.30; 4.32	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:

5.00	(organic carbon, calculated, Broman et al. 1991)
6.70	(calculated, Broman et al. 1991)
8.23	(computed-K_{OW}, Kollig 1995)
9.78; 9.76	(sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
9.92; 9.76	(GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolysis $t_{½}$ = 3.3 h in the extract from fly ash in tetradecane, for ^{13}C labelled congener (Tysklind & Rappe 1991)

$t_{½}$ = 84.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 0.92×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)

k_{OH} = $(0.5 - 0.9) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with calculated tropospheric lifetime of 17–31 d, using a 12-h average daytime OH radical concn of 1.5×10^6 molecule/cm^3 for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 42 L kg^{-1} d^{-1}, 61 L kg^{-1} d^{-1} (average k_1 for H_7CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

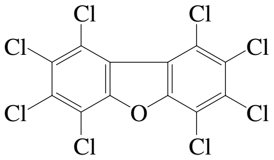
Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF, with OH radicals to be 17–31 d (Atkinson 1991);

$t_{½}$ = 3200 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{½}$ = 64 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:
Sediment: degradation $t_{½}$ = 20–200 y for all homologues (estimated, Suzuki et al. 2000);
$t_{½}$ = 300 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: degradation $t_{½}$ = 5–50 yr (estimated, Suzuki et al. 2000);
$t_{½}$ = 300 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota:

9.1.1.32 Octachlorodibenzofuran



Common Name: Octachlorodibenzofuran
Synonym: OCDF
Chemical Name: octachlorodibenzofuran
CAS Registry No: 39001-02-0
Molecular Formula: $C_6Cl_4OC_6Cl_4$
Molecular Weight: 443.753
Melting Point (°C):
258–260 (Rordorf 1986,1989)
259 (Ruelle & Kesselring 1997, Passivirta et al. 1999)
Boiling Point (°C):
510 (calculated, Rordorf 1986)
537 (calculated, Rordorf 1989)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
343.9 (calculated-Le Bas method at normal boiling point)
251.0 (Ruelle & Kesselring 1997, quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
90 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
149.43 (Rordorf 1989)
284.38 (Dickhut et al. 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
57.5 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
108 (Rordorf 1986,1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.00518 (calculated-assuming ΔS_{fus} = 56 J/mol K and mp = 258°C)
0.000037 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.16×10^{-6}* (extrapolated, generator column-GC, measured range 39.8–80°C, Doucette & Andren 1988a)
$S/(mol/L) = 2.77 \times 10^{-14} \exp(0.081 \cdot t/°C)$ (generator column-GC/ECD, temp range 40–80°C, Doucette & Andren 1988a)
$\log x = -3264/(T/K) - 2.376$, temp range 40–80°C (generator column-GC/ECD, Doucette & Andren 1988a)
1.54×10^{-6} (calculated-QSAR, Fiedler & Schramm 1990)
1.37×10^{-7} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
2.33×10^{-4}; 1.02×10^{-4} (supercooled liquid S_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
$\log [S_L/(mol/L)] = 0.5720 - 3008/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
$\ln x = -5.0496 - 7455.1/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
1.22×10^{-4}, 1.02×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
5.00×10^{-10}* (gas saturation, Rordorf 1985, 1989)
2.60×10^{-7} (supercooled liquid P_L, GC-RC correlation, Eitzer & Hites 1989)

0.000221* (105.6 °C, average value, gas saturation-GC, measured range 105.6–261.2 °C, Rordorf 1990)
5.00×10^{-10} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
1.26×10^{-9} (solid vapor pressure calculated from reported P_L, Delle Site 1997)
7.08×10^{-7}; 1.82×10^{-7} (supercooled liquid P_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
1.30×10^{-6}; 4.83×10^{-11} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 13.42 - 7073/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 7.77 - 4068/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
$\log (P/Pa) = 16.88937 - 7808.74/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.107* (165 °C, Knudsen effusion, measured range 165–195°C, Li et al. 2002)
$\log (P_L/mmHg) = 27.96 - 6148/(T/K) - 6.267 \cdot \log (T/K)$ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol or as indicated and reported temperature dependence equations):
0.10 (estimated, Clark & Mackay 1991)
1.31; 0.776 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
$\log [H/(Pa\ m^3/mol)] = 7.20 - 1060/(T/K)$ (Passivirta et al. 1999)
2.14; 0.776 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
13.06, 13.22, 13.78; 12.54, 13.37, 13.93 (HPLC-RT correlation, linear regressions; quadratic regressions, Sarna et al. 1984)
8.78 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
7.97 (generator column-GC/ECD, Doucette & Andren 1987, 1988b)
7.90 (HPLC-RT correlation, Doucette & Andren 1988b)
7.97 (recommended, Hansch et al. 1995)
8.78; 8.60 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
8.62 (calculated-solubility log S_L and regression from lit. log K_{OW}, Passivirta et al. 1999)
7.992 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
8.03; 8.60 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.84 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF:
1.613, 0.70 (human fat, calculated-different K_{OW}s, wet weight basis, Geyer et al. 1987)
1.71, 0.778 (human fat, calculated-different K_{OW}s, lipid basis, Geyer et al. 1987)
2.77; 3.89 (guppy, wet weight based; lipid weight based, Gobas & Schrap 1990)
3.90; 4.10; 4.11 (guppies, 21-d exposure, lipid wt basis: measured-C_{fish}/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
3.90; 3.88 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
7.48; 7.78 (wet wt basis: fish with 5% lipid, with 10% lipid, Geyer et al. 2000)
7.61, 7.63 (fish muscle log BCF_L calculated from water, sediment, Wu et al. 2001)
3.85; 3.88 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:
6.75 (calculated-QSAR, Fiedler & Schramm 1990)
6.00 (organic carbon, calculated, Broman et al. 1991)
7.40 (calculated, Broman et al. 1991)
7.40 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
8.13, 8.48 (calculated-K_{OW}, Kollig 1993)
10.49; 10.30 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
10.39; 10.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolytic $t_{½}$ = 2.1 h from extract of fly ash in tetradecane solution for native congener (Tysklind & Rappe 1991);

photolysis k = 2.7 × 10^{-3} min^{-1} with $t_{½}$ = 260 min in pure water and $t_{½}$ = 6.3 × 10^{-3} min^{-1} with $t_{½}$ = 110 min in 60% acetonitrile/water at 300 nm photochemical reactor; k = 0.11 h^{-1} with $t_{½}$ = 6.5 h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000).

$t_{½}$ =100.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved OCDF by ozone) is 1.05 × 10^4 L g^{-1} min^{-1} under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

k_{OH}(calc) = 0.39 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

k_{OH} = 0.4 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime τ = 39 d, using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3 for OCDF at room temp. (Atkinson 1991)

photodegradation $t_{½}$ = 9 h for OCDF adsorbed to clean silica gels in a rotary photo-reactor by filtered < 290 nm of light (Koester & Hites 1992)

Biodegradation:

Biotransformation: metabolism half-time 10^7 h (guppy, Clark & Mackay 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.012 d^{-1} (rainbow trout, Niimi & Oliver 1986)

k_1 = 824 d^{-1}; k_2 = 1.40 d^{-1} (guppy, Gobas & Schrap 1990)

k_2 = 0.0101 d^{-1} with a biological $t_{½}$ = 30 d (blue mussel, 99-d exposure, Hektoen et al. 1994)

k_1 = 217 L kg^{-1} d^{-1}; k_2 = 0.174 d^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for OCDF with OH radicals to be 39 d (Atkinson 1991);

$t_{½}$ = 9600 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis k = 2.7 × 10^{-3} min^{-1} with $t_{½}$ = 260 min in pure water and k = 6.3 × 10^{-3} min^{-1} with $t_{½}$ = 110 min in 60% acetonitrile/water at 300 nm photochemical reactor; k = 0.11 h^{-1} with a $t_{½}$ = 6.5 h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000);

$t_{½}$ = 192000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{½}$ = 29 yr (Geyer et al. 2000)

degradation $t_{½}$ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000);

$t_{½}$ = 250 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{½}$ = 5–50 yr (estimated, Suzuki et al. 2000);

$t_{½}$ = 250000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: mean biological $t_{½}$ = 7 d in rainbow trout (Niimi 1986)

$t_{½}$ = 7 to 12 d in rainbow trout (Niimi & Oliver 1986)

biological $t_{½}$ = 30 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

TABLE 9.1.32.1
Reported aqueous solubilities and vapor pressures of octachlorodibenzofuran at various temperatures

Aqueous solubility				Vapor pressure			
Doucette & Andren 1988a		Rordorf 1987, 1989		Rordorf 1990		Li et al. 2002	
generator column-GC/ECD		gas saturation-GC		gas saturation-GC		Knudsen effusion	
t/°C	$S/g{\cdot}m^{-3}$	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
39.5	3.85×10^{-6}	25	5.0×10^{-10}	105.6	0.000221	165	0.107
56.6	1.40×10^{-5}	50	5.3×10^{-8}	110.5	0.000365	170	0.160
80.0	5.86×10^{-5}	75	2.9×10^{-6}	115.5	0.000624	175	0.252
25.0	1.16×10^{-6}	100	9.1×10^{-5}	120.6	0.00109	180	0.395
	(extrapolated)	125	1.9×10^{-3}	125.5	0.00188	185	0.598
				130.5	0.00320	190	0.882
$S/(mol/L) = a{\cdot}exp[b{\cdot}(t/°C)]$		$\Delta H_V/(kJ\ mol^{-1}) = 90.0$		135.5	0.00542	195	1.240
a	5.87×10^{-13}	$\Delta H_{subl}/(kJ\ mol^{-1}) = 149.43$		140.4	0.00900		
b	0.068	$\Delta H_{fus}/(kJ\ mol^{-1}) = 57.5$		145.4	0.01475	ln P/Pa = A– B/(T/K)	
		$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1}) = 90.0$		150.5	0.02407	A	36.664 ± 0.485
$\Delta H_{sol}/(kJ\ mol^{-1}) = 53.35$				155.5	0.03853	B	17046 ± 220
	5–45°C			160.5	0.06383		
				165.6	0.09973	$\Delta H_{subl}/(kJ\ mol^{-1}) = 14172$	
				170.5	0.1540		165–195°C
				175.6	0.2393		
				180.6	0.3740		
				186.5	0.570		
				190.7	0.847		
				195.8	1.100		
				200.9	1.640		
				205.9	2.413		
				210.9	3.527		
				215.9	5.125		
				221.0	7.468		
				226.0	10.735		
				231.0	15.234		
				236.0	22.502		
				241.1	31.900		
				246.1	48.311		
				251.1	74.357		
				256.2	102.984		
				261.2	136.696		
				$\Delta H_{subl}/(kJ\ mol^{-1}) = 143.702$			
					105–261°C		

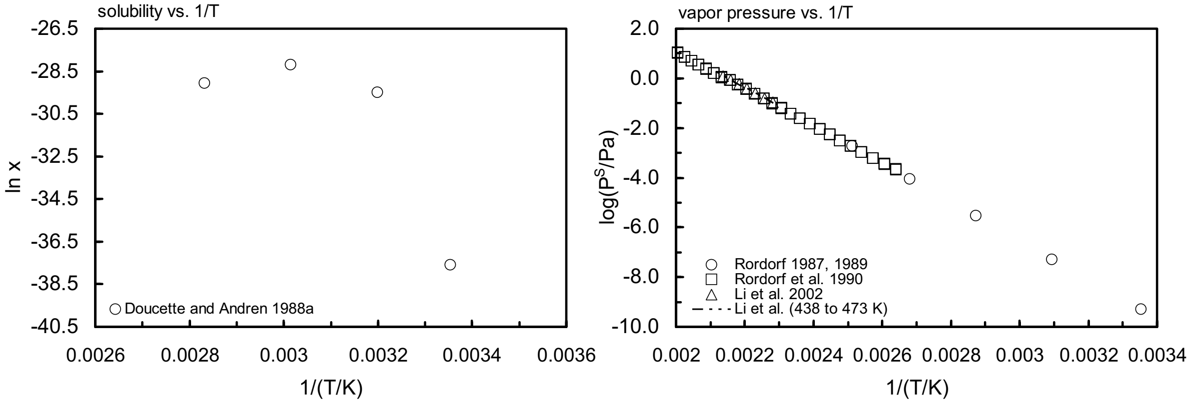


FIGURE 9.1.32.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for octachlorodibenzofuran.

9.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 9.2.1
Summary of physical properties of some chlorinated furans

Compound	CAS no.	Molecular formula	Chlorine no. n	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume V_M cm³/mol
Dibenzofuran	132-64-9	$C_{12}H_8O$	0	168.191	86.5	287	0.249	176.1
2-Chloro-	51230–49–0	$C_{12}H_7OCl$	1	202.637	101.5–102.5	338.2	0.175	197.6
3-Chloro-	25074–67–3	$C_{12}H_7OCl$	1	202.637	101–102	338.2	0.178	197.6
2,3-Dichloro-	64126–86–9	$C_{12}H_6OCl_2$	2	237.082	125.5–127	375.0	0.102	218.5
2,7-Dichloro-	73992–98–6	$C_{12}H_6OCl_2$	2	237.082				218.5
2,8-Dichloro-	5409–83–6	$C_{12}H_6OCl_2$	2	237.082	184–185	375	0.0272	218.5
3,6-Dichloro-	94570–83–9	$C_{12}H_6OCl_2$	2	237.082	188	375	0.0252	218.5
2,3,8-Trichloro-	57117–32–5	$C_{12}H_5OCl_3$	3	271.527	189–191	408.4	0.0240	239.4
2,4,6-Trichloro-	58802–14–5	$C_{12}H_5OCl_3$	3	271.527	116–117	408.4	0.126	239.4
2,4,8-Trichloro-	54589–71–8	$C_{12}H_5OCl_3$	3	271.527	154	392.5	0.0542	239.4
1,2,3,4-Tetrachloro-	24478–72–6	$C_{12}H_4OCl_4$	4	305.978	168.5–169	438.3	0.0389	260.3
1,2,3,7-Tetrachloro-	83704–22–7	$C_{12}H_4OCl_4$	4	305.978	167.5–168	438.3	0.0398	260.3
1,2,7,8-Tetrachloro-	58802–20–3	$C_{12}H_4OCl_4$	4	305.978	210–211	438.3	0.0151	260.3
1,3,6,8-Tetrachloro-	71998–72–6	$C_{12}H_4OCl_4$	4	305.978	177–178	438.3	0.0319	260.3
1,3,7,8-Tetrachloro-	57117–35–8	$C_{12}H_4OCl_4$	4	305.978				260.3
1,3,7,9-Tetrachloro-	64650–17–4	$C_{12}H_4OCl_4$	4	305.978	206.5–207.5	438.3	0.0168	260.3
2,3,7,8-Tetrachloro-	51207–31–9	$C_{12}H_4OCl_4$	4	305.978	227	438.3	0.0104	260.3
1,2,3,4,7-Pentachloro-	83704–48–7	$C_{12}H_3OCl_5$	5	340.418				281.2
1,2,3,7,8-Pentachloro-	57117–41–6	$C_{12}H_3OCl_5$	5	340.418	225–227	464.7	0.0107	281.2
1,2,4,7,8-Pentachloro-	83704–51–2	$C_{12}H_3OCl_5$	5	340.418	236–238	464.7	0.00832	281.2
2,3,4,7,8-Pentachloro-	57117–31–4	$C_{12}H_3OCl_5$	5	340.418	196–196.5	464.7	0.0209	281.2
1,2,3,4,6,8-Hexachloro-	69698–60–8	$C_{12}H_2OCl_6$	6	374.863	233.5–234	487.7	0.00895	302.1
1,2,3,4,7,8-Hexachloro-	70658–26–9	$C_{12}H_2OCl_6$	6	374.863	226	487.7	0.107	302.1
1,2,3,4,7,9-Hexachloro-	91538–84–0	$C_{12}H_2OCl_6$	6	374.863	216–217	487.7	0.0132	302.1
1,2,3,6,7,8-Hexachloro-	57117–44–9	$C_{12}H_2OCl_6$	6	374.863	232–234	487.7	0.00910	302.1
1,2,3,7,8,9-Hexachloro-	72918–21–9	$C_{12}H_2OCl_6$	6	374.863	246–249	487.7	0.00656	302.1
1,2,4,6,7,8-Hexachloro-	67562–40–7	$C_{12}H_2OCl_6$	6	374.863	221–222	487.7	0.0118	302.1
1,2,4,6,8,9-Hexachloro-	68698–59–5	$C_{12}H_2OCl_6$	6	374.863	246–248	487.7	0.00664	302.1

Continued

TABLE 9.2.1 *(continued)*

Compound	CAS no.	Molecular formula	Chlorine no. n	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume V_M cm³/mol
2,3,4,6,7,8-Hexachloro-	60851–34–5	$C_{12}H_2OCl_6$	6	374.863	239–240	487.7	0.00786	302.1
1,2,3,4,6,7,8-Heptachloro-	67462–39–4	$C_{12}HOCl_7$	7	409.308	236–237	507.2	0.00841	323.0
1,2,3,4,6,8,9-Heptachloro-	69698–58–4	$C_{12}HOCl_7$	7	409.308	211–212	507.2	0.0148	323.0
1,2,3,4,7,8,9-Heptachloro-	55673–89–7	$C_{12}HOCl_7$	7	409.308	221–223	507.2	0.0117	323.0
Octachlorodibenzofuran	39001–02–0	$C_{12}OCl_8$	8	443.753	258	537	0.00518	343.9

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 9.2.2
Selected physical-chemical properties of some chlorinated furans at 25°C

Compound	Selected properties						Henry's law const. H/(Pa·m³/mol)
	Vapor pressure		Solubility			log K_{OW}	
	P^S/Pa	P_L/Pa	S/(mg/m³)	C^S/(mmol/m³)	C_L/(mmol/m³)		calculated P/C
Dibenzofuran	0.400	1.606	4750	28.240	114.42	4.27	14.16
2,8-DCDF	0.00039	1.46×10^{-2}	14.5	0.0612	2.246	5.44	6.377
3,6-DCDF	2.00×10^{-4}	7.94×10^{-3}					
2,3,8-T_3CDF	2.48×10^{-4}	1.03×10^{-2}					
2,4,6-T_3CDF	9.22×10^{-4}	7.29×10^{-3}					
2,4,8-T_3CDF	9.1×10^{-5}	1.68×10^{-3}					
1,3,7,8-T_4CDF	3.51×10^{-5}					6.39	
2,3,7,8-T_4CDF	2.00×10^{-6}	1.92×10^{-4}	0.419	1.37×10^{-3}	0.132	6.53	1.461
2,3,4,7,8-P_5CDF	3.50×10^{-7}	1.68×10^{-5}	0.236	6.93×10^{-4}	0.0332	6.5	0.505
1,2,3,4,7,8-H_6CDF	3.20×10^{-8}	2.99×10^{-6}	0.00825	2.20×10^{-5}	2.06×10^{-3}	7.0	1.454
1,2,3,4,6,7,8-H_7CDF	4.70×10^{-9}	5.59×10^{-7}	0.00135	3.30×10^{-6}	3.92×10^{-4}	7.4	1.425
OCDF	5.0×10^{-10}	9.65×10^{-8}	0.00116	2.61×10^{-6}	5.05×10^{-5}	8.0	0.191

TABLE 9.2.3
Suggested half-life classes of polychlorinated dibenzofurans in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Dibenzofuran	3	4	6	7
2,8-Dichloro-	4	5	7	8
2,3,7,8-Tetrachloro-	4	5	8	9
2,3,4,7,8-Pentachloro-	5	5	8	9
1,2,3,4,6,7,8-Heptachloro-	5	6	8	9
Octachlorodibenzofuran	5	7	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

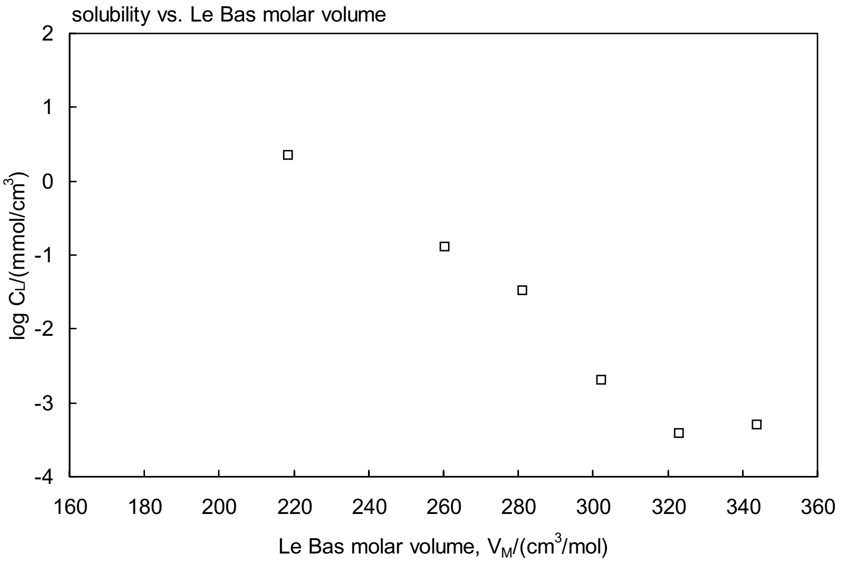


FIGURE 9.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzofurans.

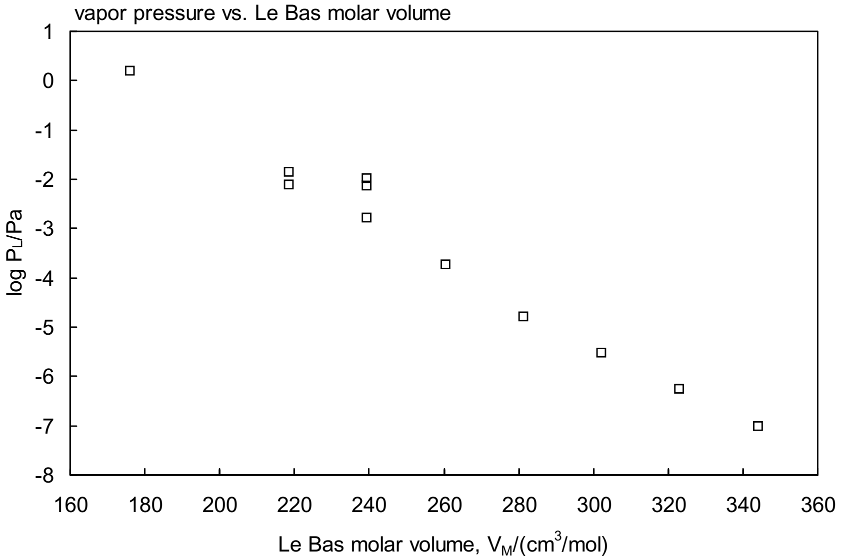


FIGURE 9.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzofurans.

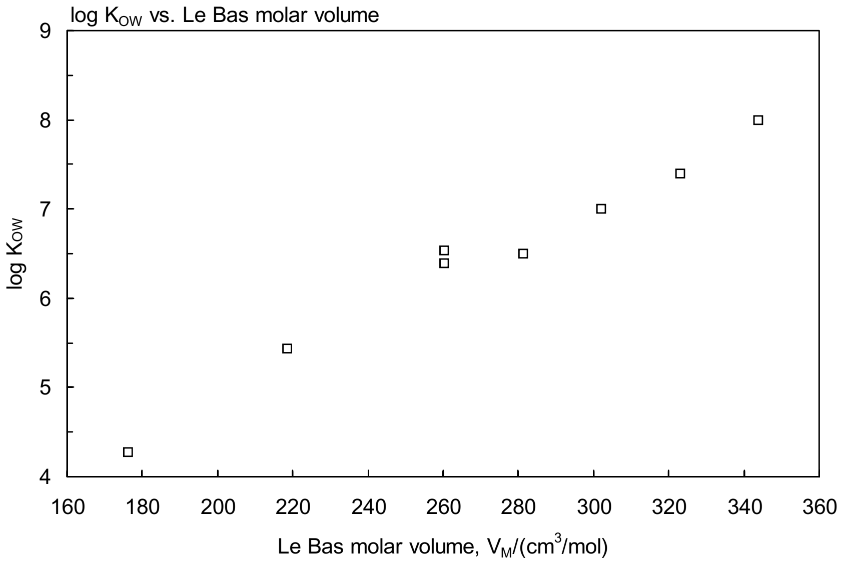


FIGURE 9.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated dibenzofurans.

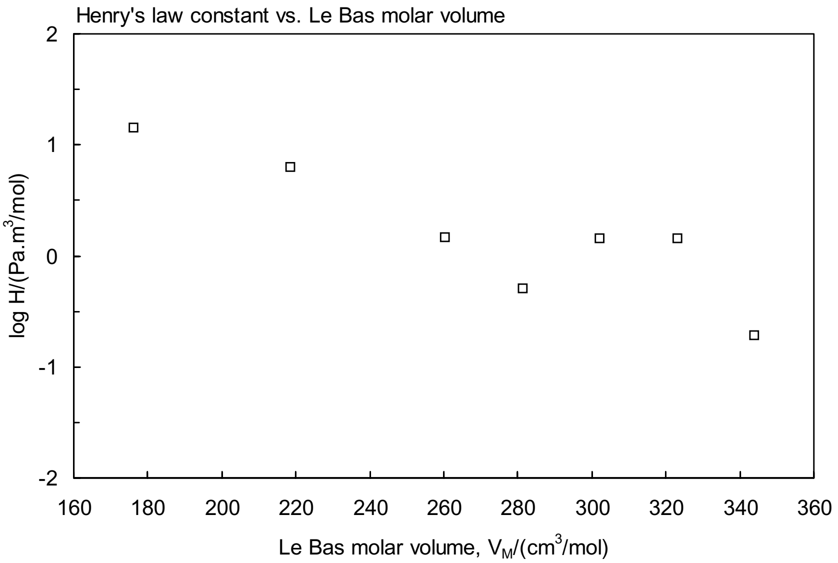


FIGURE 9.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated dibenzofurans.

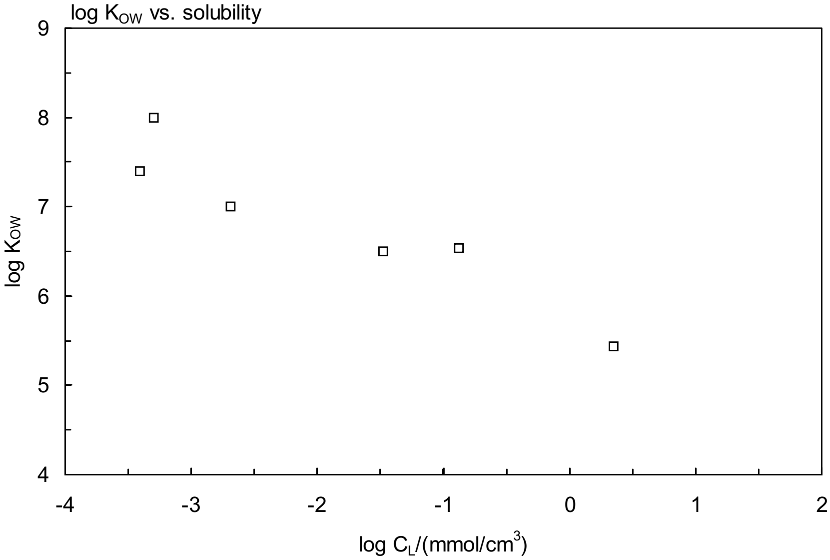


FIGURE 9.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated dibenzofurans.

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