10 Ethers

CONTENTS

10.1 LIST OF CHEMICALS AND DATA COMPILATIONS

10.1.1 Aliphatic ethers

10.1.1.1 Dimethyl ether (Methyl ether)

Common Name: Dimethyl ether
Synonym: methyl ether, oxapropane, oxybismethane
Chemical Name: dimethyl ether, methyl ether,
CAS Registry No: 115-10-6
Molecular Formula: C_2H_6O, CH_3OCH_3
Molecular Weight: 46.068
Melting Point (°C):
–138.5 (Stull 1947; Stephenson & Malanowski 1987)
–141.5 (Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
–24.75 (Ambrose et al. 1976)
–23.60 (Stephenson & Malanowski 1987)
–24.8 (Lide 2003)
Density (g/cm^3 at 20°C):
0.6689 (Riddick et al. 1986)
0.6612 (25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
68.87 (20°C, calculated-density)
60.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
4.941 (Riddick et al. 1986; Chickos et al. 1999)
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):
71000 (Seidell 1941; Lange 1971)
35.3% (24°C, selected, Riddick et al. 1986)
65200 (literature data compilation, Yaws et al. 1990)
47480 (calculated-V_M, Wang 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):
100847* (–24.91°C, static method-manometer, measured range –78.22 to –24.91°C, Kennedy et al. 1941)
678090* (calculated-Antoine eq. regression, temp range –115.7 to –23.7°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 5409.8/(T/K)] + 7.585479; temp range –115.7 to 125.2°C (Antoine eq., Weast 1972–73)
593300 (Ambrose et al. 1976, Riddick et al. 1986)
log (P/kPa) = 6.0823 – 882.52/{(T/K) + 31.90} (Antoine eq., Ambrose et al. 1976)
log (P/mmHg) = 6.97603 – 889.3645/(241.96 + t/°C); temp range –71 to –25°C (Antoine eq., Dean 1985, 1992)
log (P/kPa) = 5.44136 – 1025.56/(256.05 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
575530, 593340 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.44136 – 1025.56/(–17.1 + T/K); temp range 183–265 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.30358 – 982.46/(–20.894 + T/K), temp range not specified (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.36332 – 995.747/(–19.864 + T/K); temp range 180–249 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.09354 – 880.813/(–33.007 + T/K); temp range 241–303 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.28318 – 987.484/(–16.813 + T/K); temp range 293–360 K (Antoine eq.-V, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.48877 – 1971.127/(122.787 + T/K); temp range 349–400 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
374000* (10°C, vapor-liquid equilibrium, measured range 203.15–395 K, Noles & Zollweg 1992)
log (P/mmHg) = $20.2699 - 1.5914 \times 10^3/(T/K) - 4.653 \cdot \log (T/K) - 1.3178 \times 10^{-10} \cdot (T/K) + 2.5623 \times 10^{-6} \cdot (T/K)^2$; temp range 132–400 K (vapor pressure eq., Yaws et al. 1994)
510000* (20.5°C, vapor-liquid equilibrium, measured range 0.51–120.12°C, Jónasson et al. 1995)
589100 (25.02°C, vapor-liquid equilibrium, measured range 283.12–313.22 K, Bobbo et al. 2000)
596210* (25.022°C, static-pressure sensor, measured range 233–399 K, data fitted to Wagner type eq., Wu et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):
101.0 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
49.5, 105.7 (calculated-group contribution, calculated-bond contribution method, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:
0.10 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1987)
0.10 (recommended, Sangster 1989)
0.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
1.37 (calculated-S_{oct} 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: rate constant k, for gas-phase second order rate constants, k_{OH} 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:
$k_{O(3P)} = 5.7 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1} for the reaction with $O(_3P)$ at room temp. (Gaffney & Levine 1979)
$k_{OH}^* = 3.50 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298.9 K, measured range 298–505 K (flash photolysis-resonance fluorescence, Perry et al. 1977)
k_{OH}(calc) $= 2.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) $= 2.98 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)
$k_{NO3} \leq 3.0 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K (flash photolysis-visible absorption, Wallington et al. 1986; quoted, Sabljic & Güsten 1990; Atkinson 1991)
$k_{OH}^* = 2.95 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K, measured range 295–442 K (Tully & Droege 1987)
$k_{NO3} = 2.92 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Sabljic & Güsten 1990)
k_{OH}(exptl) $= 2.98 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) $= 1.98 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
$k_{OH}^* = (24.9 \pm 2.2) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988b)
$k_{OH} = 2.49 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}; k(soln) $= 1.7 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988a)
$k_{OH}^* = 2.98 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989, 1990)
$k_{OH} = (2.35 \pm 0.24) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by pulse radiolysis-UV spectroscopy; $k_{OH} = (3.19 \pm 0.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)
$k_{OH}^* = 2.95 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K, measured range 295–650 K (laser photolysis-laser induced fluorescence technique, Arif et al. 1997)

k_{OH}* = 2.86 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 263–351 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance $t_{½}$ < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); calculated lifetimes of 4.1 d and 180 d for reactions with OH radical, NO_3 radical, respectively (Atkinson .2000)

TABLE 10.1.1.1.1

Reported vapor pressures of dimethyl ether 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)		
log P = A – B/(T/K) + C·log (T/K) – D·(T/K)	(5)		

1.

Kennedy et al. 1941		Stull 1947		Jónasson et al. 1995		Wu et al. 2004	
static method-manometer		summary of literature data		static-pressure gauge		quartz pressure sensors	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–78.22	4684	–115.7	133.3	0.51	270000	233.128	54610
–70.66	8121	–101.1	666.6	3.07	300000	238.126	68490
–65.25	11706	–93.3	1333	4.97	330000	243.157	85570
–60.03	16315	–85.2	2666	15.01	430000	248.152	105590
–55.14	21910	–76.2	5333	20.50	510000	253.152	129.42
–49.90	29585	–70.4	7999	27.11	630000	258.160	157530
–45.10	38334	–62.7	13332	33.39	750000	263.160	190440
–40.02	49810	–50.0	26664	44.39	990000	268.161	228480
–35.10	63401	–37.8	53329	50.25	1160000	273.153	272170
–27.67	89362	–23.7	101325	63.94	1590000	278.145	321870
–24.91	100847			76.67	2080000	283.160	378660
		mp/°C	–138.5	89.25	2680000	288.174	444570
mp/°C	–141.5			103.77	3500000	293.161	515530
bp/°C	–24.82			120.12	4720000	298.172	596210
		Noles & Zollweg 1992				303.160	687370
eq. 5	P/mmHg	vapor-liquid equilibrium				305.160	726260
A	23.686185	t/°C	P/Pa			308.158	787070
B	1691.8056	10	37400			313.156	897590
C	–6.04560	50	114900			316.154	968550
D	0.00195754	90	273800			318.158	1018910
temp range 195–284.34 K		99.95	328400			323.149	1152350
		109.85	357000			328.149	1298230
		121.85	488200			333.157	1457500
						more to	
						400.378	5355800
						data fitted to Wagner eq.	

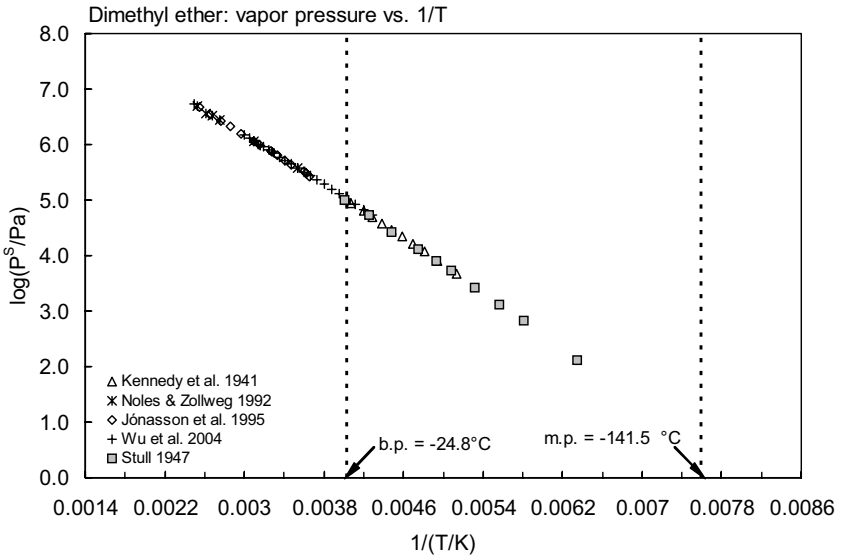
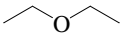


FIGURE 10.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl ether.

10.1.1.2 Diethyl ether (Ethyl ether)



Common Name: Diethyl ether
Synonym: ether, ethyl ether, ethoxyethane, ethyl oxide, 3-oxapentane, 1,1′-oxybisethane, sulfuric ether
Chemical Name: ether, diethyl ether, ethoxyethane, ethyl oxide, 3-oxapentane, 1,1′-oxybisethane
CAS Registry No: 60-29-7
Molecular Formula: $C_4H_{10}O$, $CH_3CH_2OCH_2CH_3$
Molecular Weight: 74.121
Melting Point (°C):
–116.2 (Lide 2003)
Boiling Point (°C):
34.5 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 20°C):
0.7136. 0.7078 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
103.9 (20°C, calculated-density)
106.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
5.439 (quoted, Riddick et al. 1986)
7.19 (exptl., Chickos et al. 1999)
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):
60270* (thermostatic volumetric method, measured range –3.83 to 30°C, Hill 1923)
60400* (volumetric method, measured range 10–30°C, Kablukov & Malischeva 1925)
60300* (volumetric method, measured range 10–25°C, Bennett & Phillip 1928)
69000 (Seidell 1941; Lange 1971)
60400 (selected, Riddick et al. 1986)
60900 (literature data compilation, Yaws et al. 1990)

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):
58335* (19.871°C, manometer, measured range –60.799–19.871°C, Taylor & Smith)
74690* (calculated-Antoine eq. regression, temp range –74 to 35.6°C, Stull 1947)
323835* (71.11°C, static method-Bourdon, measured range 71.11–187.78°C, Kobe et al. 1956)
log (P/mmHg) = [–0.2185 × 6946.2/(T/K)] + 7.56659; temp range –74.3 to 183.3°C (Antoine eq., Weast 1972–73)
58920 (20°C, Verschueren 1983)
63340* (21.82°C, ebulliometry, measured range 250–467 K, Ambrose et al. 1972; quoted, Boublik et al. 1984)
log (P/kPa) = 6.05115 – 1062.409/[(T/K) – 44.967]; temp range 250–329 K (ebulliometry, Antoine eq., Ambrose et al. 1972)
71620 (Ambrose et al. 1976)
71240, 71610 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.04972 – 1066.052/(220.003 + t/°C); temp range –70.0 to 19.87°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.0492 – 1061.391/(228.06 + t/°C); temp range –23.1 to 55.434°C (Antoine eq. from reported exptl. data of Ambrose et al. 1972, Boublik et al. 1984)
log (P/mmHg) = 6.92032 – 1064.07/(228.8 + t/°C); temp range –61 to 20°C (Antoine eq., Dean 1985, 1992)
71620 (selected, Riddick et al. 1986)

log (P/kPa) = 6.05115 – 1062.409/(228.183 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
71620, 71604 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.02962 – 1051.432/(–44.967 + T/K); temp range 286–329 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.05115 – 1062.409/(–44.967 + T/K); temp range 250–329 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.30714 – 1236.75/(–20.11 + T/K); temp range 307–457 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.05933 – 1067.576/(–44.217 + T/K); temp range 305–360 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.37811 – 1276.822/(–14.869 + T/K); temp range 417–467 K (Antoine eq.-V, Stephenson & Malanowski 1987)
log (P/mmHg) = 41.7519 – 2.741×10^3/(T/K) – 12.27·log (T/K) – 3.1948×10^{-10}·(T/K) + 5.9802×10^{-6}·$(T/K)^2$; temp range 157–467 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence):

130 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
90.0 (calculated-group contribution method, Hine & Mookerjee 1975)
237 (calculated-bond contribution method, Hine & Mookerjee 1975)
87.9 (calculated-P/C using Riddick et al. 1986 data)
86.8 (23°C, batch air stripping-IR, Nielsen et al. 1994)
95.05 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 5.953 – 2158/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.83 (20°C, shake flask-CR, Collander 1951)
1.03 (Hansch et al. 1968)
0.89 (shake flask-GC, both phases, Hansch et al. 1975)
0.77 (shake flask, Log P Database, Hansch & Leo 1987)
0.89 (recommended, Sangster 1989)
0.89 (recommended, Hansch et al. 1995)

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

2.19 (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, $t_{½}$:

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) = 1.43×10^{-11} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.34×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_{OH}* = 13.4×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 295 K, measured range 295–442 K (Tully & Droege 1987)
k_{OH}(exptl) = 1.34×10^{-11} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 1.06×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_{OH}* = $(13.6 \pm 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988b)
k_{OH} = 1.36×10^{-11} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 6.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988a)
k_{OH} = 1.20×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 294 K (relative rate method, Bennett & Keer 1989)
k_{OH}* = 1.33×10^{-11} cm^3 $molecule^{-1}$ s^{-1} 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (11.3 \pm 0.10) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by pulse radiolysis-UV spectroscopy; $k_{OH} = (12.8 \pm 0.6) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance $t_{½} < 0.24$ h from the air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
calculated lifetimes of 11 h and 17 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

TABLE 10.1.1.2.1
Reported aqueous solubilities of diethyl ether at various temperatures

Hill 1923		Kablukov & Malischeva 1925		Bennett & Phillip 1928	
volumetric method		volumetric method		volumetric method	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
–3.83	127520	10	90100	10	91000
0	116680	15	78700	15	79500
10	90400	20	68800	20	68700
15	79130	25	60400	25	60300
20	68960	30	53400		
25	60270				
30	53400				

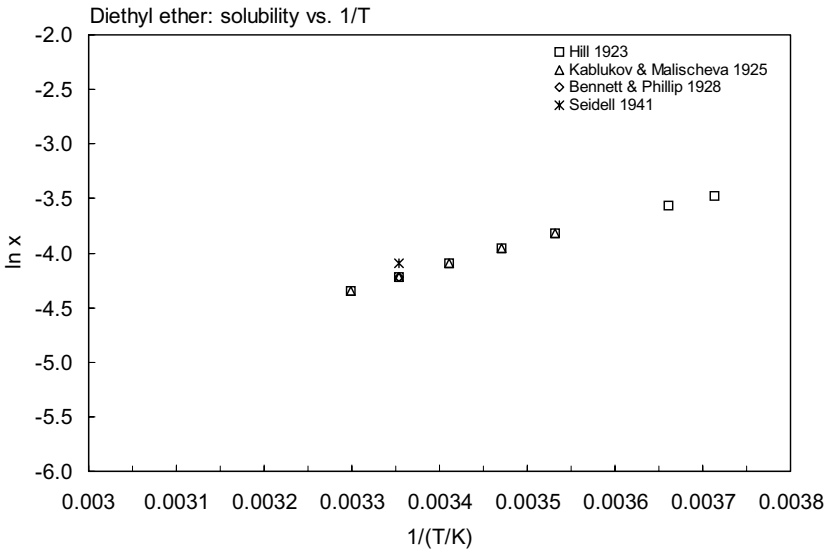


FIGURE 10.1.1.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for diethyl ether.

TABLE 10.1.1.2.2
Reported vapor pressures of diethyl ether 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)		

Taylor & Smith 1922		Stull 1947		Kobe et al. 1956		Ambrose et al. 1972	
manometer		summary of literature data		static method-Bourdon gauge		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–60.799	527	–20.4	133.3	71.11	323835	–23.104	7430
–55.748	791	–3.0	666.6	76.67	372065	–19.889	8933
–50.873	1169	5.5	1333	82.22	427186	–16.744	10619
–45.998	1683	14.3	2666	87.78	496087	–13.492	12664
–41.125	2370	24.5	5333	93.33	564988	–10.135	15090
–36.231	3302	31.0	7999	98.89	647669	–6.929	17753
–31.329	4537	39.8	13332	104.44	730351	–2.762	21778
–26.421	6107	52.7	26664	110.00	826812	0.828	25813
–21.502	8174	68.0	53329	115.56	923273	4.912	31134
–16.578	10755	82.9	101325	121.11	1040405	8.914	37179
–11.637	13971			126.67	1157537	13.137	44534
–6.698	17966	mp/°C	25.3	132.22	1288449	17.785	53941
0.009	24815			137.78	1426251	21.821	63.343
4.975	31161			143.33	1584723	26.115	74719
9.937	38746			148.89	1743195	30.764	88.801
14.093	47749			154.44	1929288	34.321	100931
19.871	58335			160.00	2122151	35.064	103618
				165.56	2287513	39.222	119720
				171.11	2542447	42.978	135889
				176.67	2797381	47.470	157395
				182.22	3059204	51.765	180321
				187.78	3341699	55.434	201878
						eq. 3	P/kPa
						A	6.05115
						B	1062.409
						C	–44.967

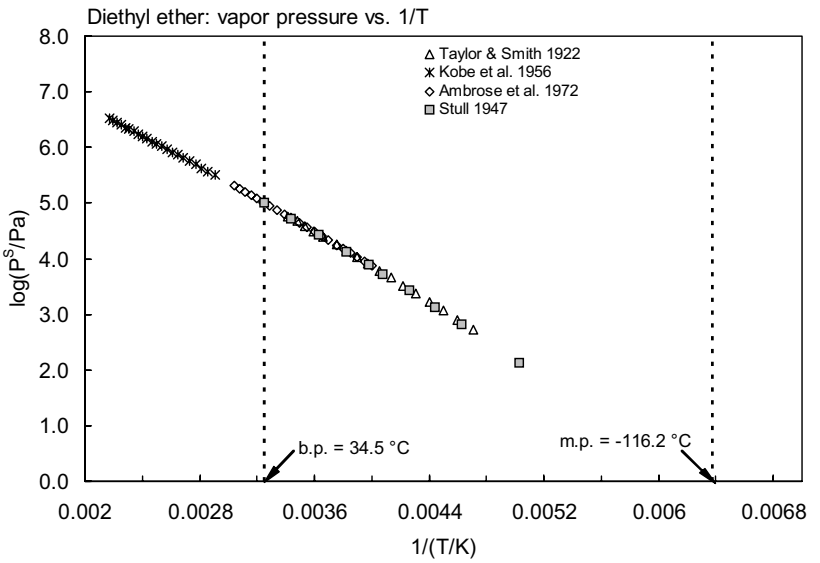


FIGURE 10.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for diethyl ether.

10.1.1.3 Methyl *t*-butyl ether (MTBE)

Common Name: Methyl *t*-butyl ether
Synonym: MTBE, 3-oxa-3,3-dimethylbutane, 2-methoxy-2-methyl-propane
Chemical Name: methyl *tert*-butyl ether
CAS Registry No: 1634-04-4
Molecular Formula: $C_5H_{12}O$, CH_3-O-$C(CH_3)_3$
Molecular Weight: 88.148
Melting Point (°C):
–108.6 (Lide 2003)
Boiling Point (°C):
55.0 (Lide 2003)
Density (g/cm^3 at 20°C):
0.7578 (Bennett & Phillip 1928)
0.7404 (Windholz 1983; Budavari 1989)
Molar Volume (cm^3/mol):
119.1 (20°C, calculated-density)
127.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
7.60 (exptl., Chickos et al. 1999)
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):
51600* (thermostatic volumetric method, measured range 0–25°C, Bennett & Phillip 1928)
48000 (Windholz 1983; Budavari 1989)
52100 (literature data compilation, Yaws et al. 1990)
42000* (19.8°C, shake flask-GC/TC, measured range 0–48.6°C, Stephenson 1992)
62100, 35500 (5, 20°C, shake flask-GC, Fischer 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):
31156* (23.243°C, comparative ebulliometry, measured range 288–351 K, Ambrose et al. 1976)
log (P/kPa) = 6.09379 – 1173.036/{(T/K) + 41.366}; temp range 288–351 K (Antoine equation, comparative ebulliometry, Ambrose et al. 1976)
32660 (Windholz 1983; Budavari 1989)
33545 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.09111 – 1171.54/(–41.542 + T/K); temp range 287–351 K (Antoine eq., Stephenson & Malanowski 1987)
37417* (27.806°C, static method, measured range 301–411 K, Krähenbühl & Gmehling 1994)
log (P/kPa) = 6.070343 – 1158.923/(T/K) – 43.20; temp range 301–411 K (Antoine eq., static method, Krähenbühl & Gmehling 1994
log (P/mmHg) = 4.7409 – 1.9493 × 10^3/(T/K) + 3.077·log (T/K) – 1.4463 × 10^{-2}·(T/K) + 1.0039 × 10^{-5}·$(T/K)^2$; temp range 165–497 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section):
59.46 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
142.6, 305 (calculated-group contribution, calculated-bond contribution method, Hine & Mookerjee 1975)
53.54*, 121 (25, 30°C, static headspace-GC, Robbins et al. 1993)
63.2 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

137.6* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)
ln K_{AW} = 6.6475 – 2901.4/(T/K); temp range 15–40°C (SPME-GC, Bierwagen & Keller 2001)
41.2 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 9.070 – 3178/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
72.4* (equilibrium concentration ratio-GC, measured range 3–25°C, Fischer et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
1.06 (Hansch et al. 1968; Kier & Hall 1976)
1.30 (calculated-fragment const., Hansch & Leo 1979)
0.94 (shake flask-GC, Funasaki et al. 1985)
0.94 (recommended, Sangster 1989)
0.94 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant, 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}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 2.64×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)
k_{OH}(exptl) = 2.64×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 1.4×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_{OH}* = $(3.09 \pm 0.15) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)
k_{OH} = 3.09×10^{-12} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 2.7×10^{-12} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)
k_{OH}* = 2.83×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
k_{OH} = $(2.44 – 3.09) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295–298 K (Atkinson 1989)
k_{OH}* = 2.98×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 293 K, measured range 293–750 K (laser photolysis-laser induced fluorescence technique, Arif et al. 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: disappearance $t_{½}$ < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
calculated lifetimes of 3.9 d and 72 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

TABLE 10.1.1.3.1
Reported aqueous solubilities of methyl *tert*-butyl ether (MTBE) at various temperatures

Bennett & Phillip 1928		Stephenson 1992		Fischer et al. 2004	
volumetric method		shake flask-GC/TC		shake flask-GC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	91200	0	83000	5	62100
10	73000	9.7	51000	20	35500
15	65500	19.8	42000		
20	58300	29.6	31000		
25	51600	39.3	25000		
		48.6	19000		

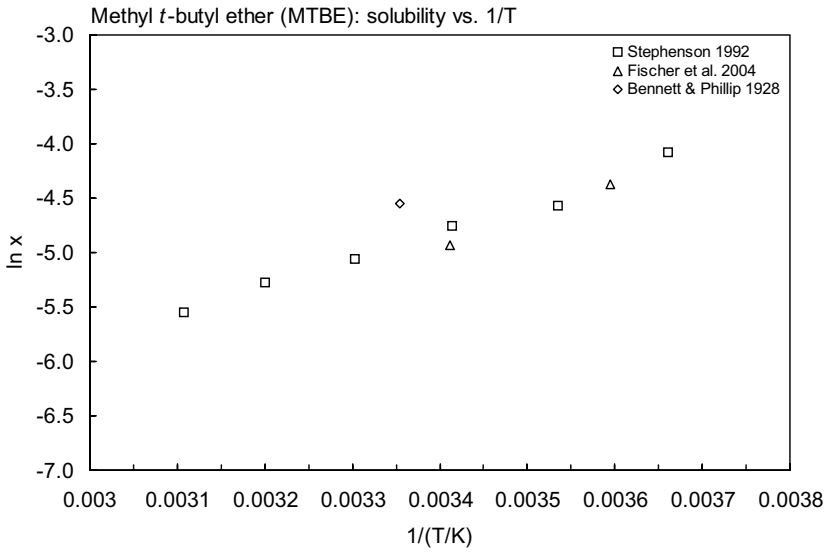


FIGURE 10.1.1.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

TABLE 10.1.1.3.2
Reported vapor pressures of methyl *tert*-butyl ether (MTBE) at various temperatures

Ambrose et al. 1976				Krähenbühl & Gmehling 1994			
comparative ebulliometry				static method*			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
14.847	21805	73.873	180280	300.956	37417	342.570	158286
18.83	25843	77.828	201818	304.397	42944	342.592	158403
23.243	31156	25	33530	307.896	49188	342.652	158669
27.518	37194			312.707	58733		
32.143	44576	log P = A – B/(C + t/°C)		318.586	72841	*complete list see ref.	
37.16	53942		P/mmHg	323.663	86748		
41.525	63351	A	6.09379	323.666	86855		
44.835	71313	B	1173.036	328.498	102046		
51.182	88805	C	−41.366	328.528	102133		
55.028	100933	bp	328.30 K	333.387	119445		
55.826	103610			333.386	119444		
60.318	119700	coefficients of		338.224	138873		
64.376	135835	also given in text		338.229	138893		
69.193	157164			338.232	138905		

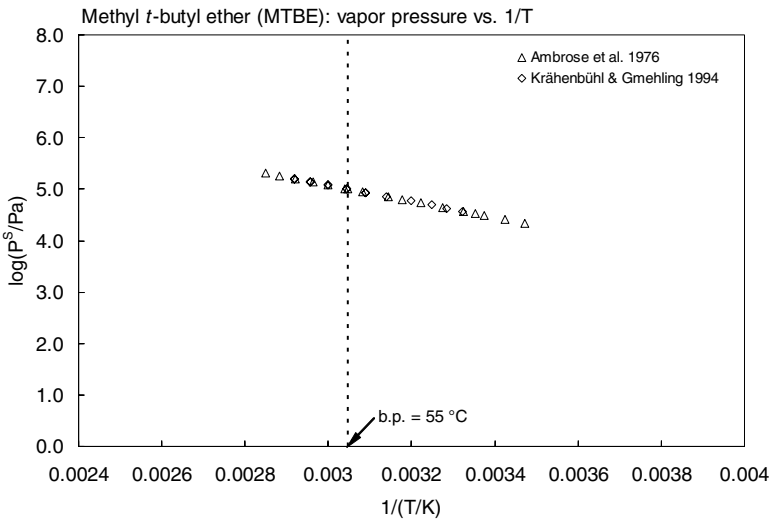


FIGURE 10.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

TABLE 10.1.1.3.3
Reported Henry's law constants of methyl *tert*-butyl ether (MTBE) 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)		
$\ln [H/(Pa\ m^3/mol)] = A - B/(T/K)$	(4)	$\ln [H/(atm \cdot m^3/mol)] = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

Robbins 1993		Bierwagen & Keller 2001		Fischer et al. 2004	
static headspace-GC		SPME-GC		equilibrium concn ratio-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
25	53.5	15	93.2	3	20.9
30	120.6	25	137.6	5	25.9
40	223.9	30	179.2	10	27.5
45	367.8	40	222.0	15	42.4
50	413.4			20	54.6
		eq. 1a	K_{AW}	25	72.4
eq. 1	H/(atm m³/mol)	A	6.6475		
A	18.4	B	3178		
B	7666				

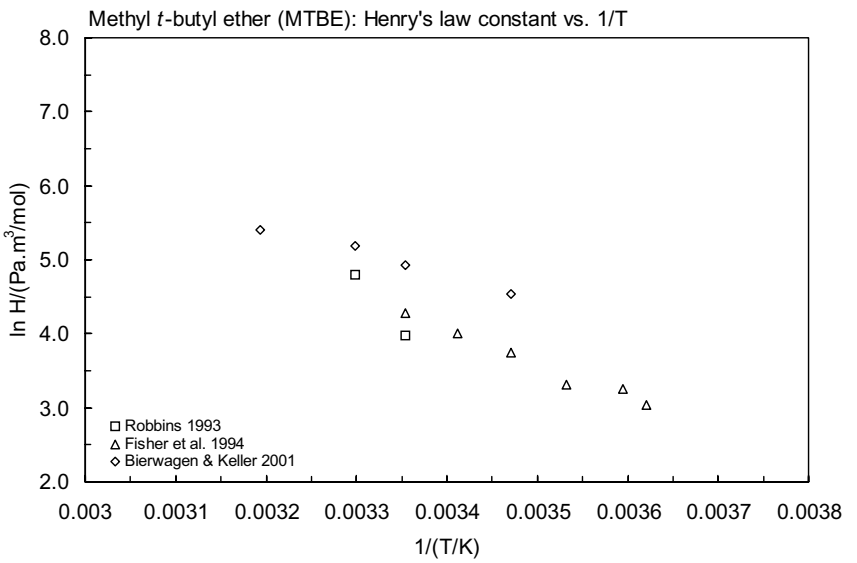
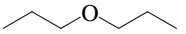


FIGURE 10.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

10.1.1.4 Di-*n*-propyl ether



Common Name: Di-*n*-propyl ether
Synonym: 4-oxaheptane, 1,1′-oxibispropane, 1-propoxypropane, propyl ether
Chemical Name: di-*n*-propyl ether, propyl ether, 4-oxaheptane
CAS Registry No: 111-43-3
Molecular Formula: $C_6H_{14}O$, $(n\text{-}C_3H_7)_2O$
Molecular Weight: 102.174
Melting Point (°C):
–114.8 (Lide 2003)
Boiling Point (°C):
90.08 (Riddick et al. 1986; Lide 2003)
Density (g/cm^3 at 20°C):
0.7466, 0.7419 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
136.9 (20°C, calculated-density)
151.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
10.78 (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):
4900* (thermostatic volumetric method, measured range 0–25°C, Bennett & Phillip 1928)
2500* (synthetic method, measured range 0–25°C, Bennett & Phillip 1928)
3000 (Seidell 1941; Lange 1971)
2508 (selected, Hine & Mookerjee 1975)
4900 (selected, Riddick et al. 1986)
3820 (literature data compilation, Yaws et al. 1990)

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):
9072* (calculated-Antoine eq. regression, temp range –43.3 to 89.5°C, Stull 1947)
16358* (39.703°C, comparative ebulliometry, measured range 39.703–98.183°C, Meyer & Hotz 1973)
log (P/mmHg) = [–0.2185 × 8229.6/(T/K)] + 7.863332; temp range –43.3 to 89.5°C (Antoine eq., Weast 1972–73)
9041* (26.59°C, ebulliometry, measured range 26.59–88.65°C, Cidlinski & Polak 1969; quoted, Boublik et al. 1984)
log (P/cmHg) = 5.894812 – 1227.468/(215.7007 + t/°C); temp range 39.7–98.2°C (comparative ebulliometry, Meyer & Hotz 1973)
7621* (23.174°C, ebulliometry, measured range 292.974–387.883 K, Ambrose et al. 1976)
log (P/kPa) = 6.03075 – 1233.148/{(T/K) + 56.708}; temp range 293–388 K (Antoine eq., ebulliometry, Ambrose et al. 1976)
8378, 8320 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.06887 – 1254.429/(218.781 + t/°C); temp range 26.59–88.65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.01902 – 1227.068/(215.654 + t/°C); temp range 39.7–86.18°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9476 – 1256.5/(219.0 + t/°C); temp range 26–89°C (Antoine eq., Dean 1985, 1992)
8334 (selected, Riddick et al. 1986)
log (P/kPa) = 6.03075 – 1133.748/(216.442 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
8334 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.019715 – 1227.468/(–57.449 + T/K); temp range 312–371 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.0361 – 1236.828/(–56.358 + T/K); temp range 292–389 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.50879 – 1579.466/(–12.142 + T/K); temp range 385–467 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 8.20381 – 3494.323/(209.259 + T/K); temp range 465–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P/mmHg) = 44.0232 – 3.282×10^3/(T/K) – 12.792·log (T/K) + 1.2682×10^{-10}·(T/K) + 4.8776×10^{-6}·$(T/K)^2$; temp range 150–531 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

350.1 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
175.5, 594.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
223.3 (computer value, Yaws et al. 1991)

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

2.03 (shake flask, Hansch et al. 1968; Leo et al. 1971)
2.03 (recommended, Sangster 1989)
2.03 (recommended, Hansch et al. 1995)

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

2.97 (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, $t_{½}$:

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:
$k_{OH} = 1.68 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (relative rate, Lloyd et al. 1976)
k_{OH}(calc) = 2.05×10^{-11} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.68×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)
k_{OH}(calc) = 1.57×10^{-11} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = 1.68×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_{OH}* = $(18.0 \pm 2.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)
$k_{OH} = 1.53 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 294 ± 2 K (relative rate method, Bennett & Kerr 1989)
k_{OH}* = 1.72×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
$k_{OH} = (19.9 \pm 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by pulse radiolysis-UV spectroscopy; $k_{OH} = (20.3 \pm 1.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½}$ < 0.24 h from air) for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.1.4.1
Reported aqueous solubilities of di-*n*-propyl ether at various temperatures

Bennett & Phillip 1928			
volumetric method		synthetic method	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	10500	0	5800
10	7100	10	4100
15	6100	15	3800
20	5400	20	3000
25	4900	25	2500

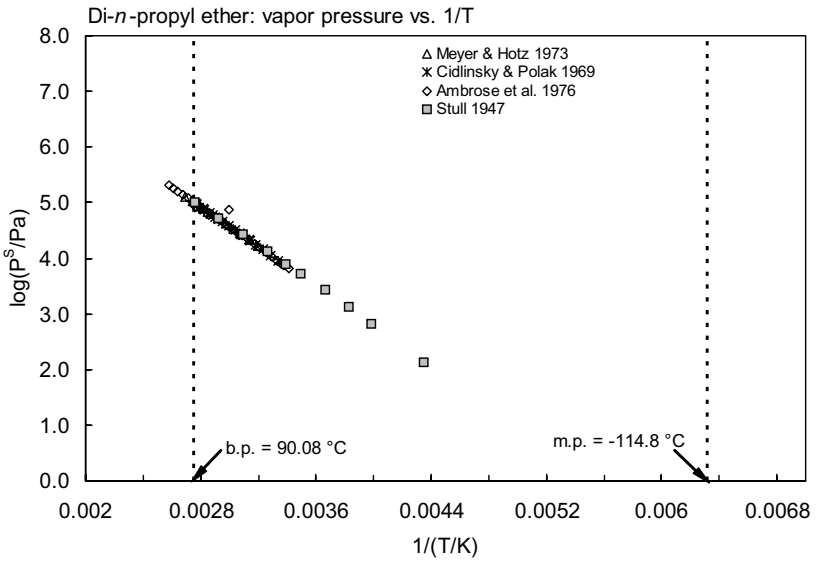


FIGURE 10.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-propyl ether.

TABLE 10.1.1.4.2
Reported vapor pressures of di-*n*-propyl ether at various temperatures and the coefficients for the vapor pressure equations

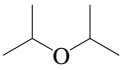
log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		
log P = A = [1 – T_B/T)]	(5)	where log A= = (a + bT + CT^2)	

Stull 1947		Meyer & Hotz 1973		Cidlinsky & Polak 1969		Ambrose et al. 1976	
summary of literature data		comparative ebulliometry		Boublik et al. 1984		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–43.3	133.3	39.703	16358	26.59	9041	19.824	6442
–22.3	666.6	45.857	21223	31.42	11344	23174	7621
–11.8	1333	51.773	26.953	36.48	14271	26.887	9130
0	2666	57.749	33962	40.83	17252	30.501	10829
13.2	5333	63.263	41649	45.08	20.662	34.27	12873
21.6	7999	69.298	51617	46	21463	38.124	15283
33	13332	75.199	63121	50.47	25724	41.833	17938

TABLE 10.1.1.4.2 (*Continued*)

Stull 1947		Meyer & Hotz 1973		Cidlinsky & Polak 1969		Ambrose et al. 1976	
summary of literature data		comparative ebulliometry		Boublik et al. 1984		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
50.3	26664	77.936	69101	52.94	28338	46.698	21992
69.5	53329	81.601	77811	55.89	31760	50.87	26026
89.5	101325	84.221	84548	60.7	38035	55.827	31341
		91.016	104174	65.98	46095	60.296	37380
mp/°C	–112	98.183	128564	68.76	50822	65.228	44739
				71.44	55747	70.661	54144
		bp/°C	340.096	73.77	60355	75.383	63545
				76.27	65592	60.404	74921
		constants for Antoine eq.		80.49	76152	85.849	89008
		eq. 2	P/cmHg	82.13	79460	90.007	101105
		A	5.894812	85.77	83202	95.743	119879
		B	1227.468	87.34	93648	100.145	136045
		C	215.707	88.65	97250	105.407	157559
		temp range: 39.7–58.2°C				110.436	180476
				eq. 2	P/kPa	114.733	202031
		constants for Cox eq.		A	6.06887	25	8334
		eq. 5	P/atm	B	1254.429		
		a	0.866715	C	216.781	eq. 2	P/kPa
		$-b \times 10^3$	0.812825	bp/°C	89.952	A	6.03075
		$b \times 10^6$	0.809693			B	1233.748
		T_B/K	364.2462			C	–56.708
						coefficients of Chebyshev eq. also given in text	

10.1.1.5 Di-isopropyl ether



Common Name: Di-isopropyl ether
Synonym: diisopropyloxyde, isopropyl ether, 2-isopropoxypropane, 2,2′-oxybispropane, 3-oxa-2,4-dimethylpentane, IPE, DIPE
Chemical Name: diisopropyl ether, isopropyl ether, 2-isopropoxypropane, 2,2′-oxybispropane, 3-oxa-2,4-dimethylpentane
CAS Registry No: 108-20-3
Molecular Formula: $C_6H_{14}O$, $[(CH_3)_2CH]_2O$
Molecular Weight: 102.174
Melting Point (°C):
–85.4 (Lide 2003)
Boiling Point (°C):
68.4 (Lide 2003)
Density (g/cm^3 at 20°C):
0.7360 (Bennett & Phillip 1928)
0.7239, 0.7185 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
140.0 (20°C, calculated-density)
151.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
12.033 (quoted, Riddick et al. 1986)
12.05 (exptl., Chickos et al. 1999)
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):
2040 (selected, Hine & Mookerjee 1975)
9000 (20°C, Verschueren 1983)
12000 (20°C, selected, Riddick et al. 1986)
11200 (literature data compilation, Yaws et al. 1990)
7900*, 5400 (20°C, 31°C, shake flask-GC/TC, measured range 0–61°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):
21410* (calculated-Antoine eq. regression, temp range –57 to 67.5°C, Stull 1947)
log (P/mmHg) = 7.09712 – 1257.6/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
20093* (temp range 0–60°C, Nicolini & Laffitte 1949)
21532* (26.8°C, ebulliometry, measured range 13.5–70.6°C, Flom et al. 1951)
20194* (25.29°C, ebulliometry, measured range 23.5–67.21°C, Cidlinsky & Polak 1969; quoted, Boublik et al. 1984)
log (P/mmHg) = [–0.2185 × 7777.3/(T/K)] + 7.904664; temp range –57 to 67.5°C (Antoine eq., Weast 1972–73)
17778* (22.489°C, ebulliometry, measured 284.779–365.122 K, Ambrose et al. 1976)
log (P/kPa) = 5.97678 – 1143.073/{(T/K) + 53.810}; temp range 284–365 K (Antoine eq., ebulliometry, Ambrose et al. 1976)
19954, 20120 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.78384 – 1050.657/(209.511 + t/°C); temp range 0–60°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 5.97081 – 1137.408/(218.516 + t/°C); temp range 23.5–67.21°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.8495 – 1139.34/(218.7 + t/°C); temp range 23–67°C (Antoine eq., Dean 1985, 1992)

19880 (selected, Riddick et al. 1986)
log (P/kPa) = 5.97678 – 1143.073/(219.340 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
19950, 19890 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.966496 – 1135.034/(–54.92 + T/K); temp range 296–342 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.97661 – 1142.985/(–53.82 + T/K); temp range 284–365 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.26597 – 1334.298/(–28.271 + T/K); temp range 360–440 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.13537 – 2140.415/(80.78 + T/K); temp range 436–500 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
19862, 10850 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
log (P/mmHg) = 35.9552 – 2.0276×10^3/(T/K) –2.8551·log (T/K) + 2.7662×10^{-4}·(T/K) – 9.9111×10^{-14}·$(T/K)^2$; temp range 188–500 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
1010 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
483.3, 594.6 (calculated-group contribution calculated-bond contribution, Hine & Mookerjee 1975)
175.6 (computer value, Yaws et al. 1991)
208.8 (23°C, batch air stripping-IR, Nielsen et al. 1994)
212.4 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
231 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
1.52 (shake flask-GC, Funasaki et al. 1985)
1.56 (calculated-fragment const., Hansch & Leo 1979)
1.52 (recommended, Sangster 1989)
1.52 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
2.66 (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, $t_{½}$:
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:
$k_{OH} = (1.07 \pm 0.20) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} by pulse radiolysis-UV spectroscopy, $k_{OH} = (1.13 \pm 0.20) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K by relative rate technique (Nelson et al. 1990)
$k_{OH}^* = (1.08 \pm 0.09) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 240–400 K (absolute rate, flash photolysis-resonance fluorescence, Wallington et al.1993)
$k_{OH} = (9.9 \pm 0.2) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} and $(1.07 \pm 0.6 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (relative rate method, Wallington et al.1993)
$k_{OH} = 9.8 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K using both relative (at 295 K) and absolute techniques over 240–440 K (FT-IR spectroscopy, Wallington et al. 1993)
$k_{OH} = 2.2 \times 10^{-12}$ exp[(445 ± 1450)/(T/K)]; temp range 240–440 K (Arrhenius eq., FT-IR, Wallington et al. 1993)
k_{OH}(calc) = 33.3×10^{-12} cm^3 mol^{-1} s^{-1}, k_{OH}(exptl) = 10.2×10^{-12} cm^3 mol^{-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 $t_{½} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.5.1
Reported aqueous solubilities of di-isopropyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	**S/g·m^{-3}**
0	22800
9.7	10200
20	7900
31	5400
40.8	4100
50.7	2800
61	2200

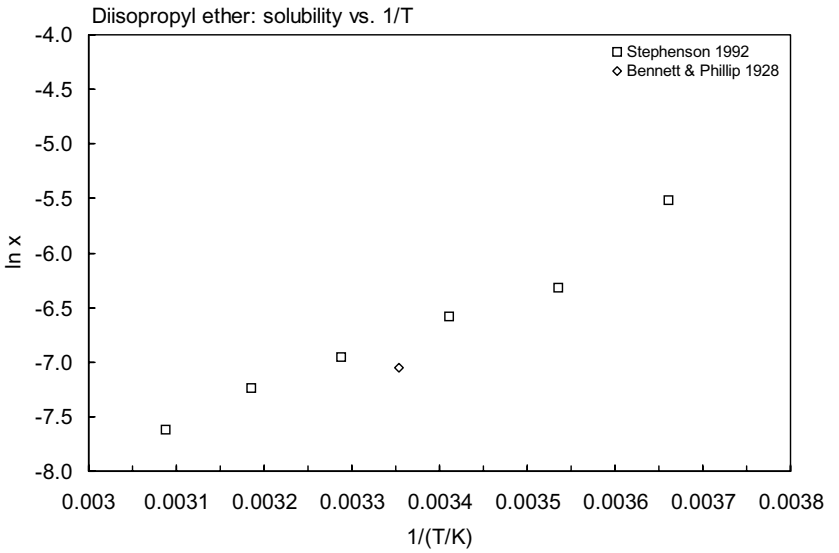


FIGURE 10.1.1.5.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for di-isopropyl ether.

TABLE 10.1.1.5.2
Reported vapor pressures of di-isopropyl ether 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
summary of literature data

t/°C	P/Pa
–57.0	133.3
–37.4	666.6
–27.4	1333
–16.7	2666
–4.50	5333
3.4	7999
13.7	13332
30	26664
48.2	53329
67.5	101325
mp/°C	–60.0

Flom et al. 1951
dynamic-ebulliometry

t/°C	P/Pa
13.5	11466
26.8	21532
35.1	30491
42.4	40423
47.9	50356
53	60062
56.7	68541
59.8	76354
63	85380
66.3	95859
69.5	104205
70.6	109471

Nicolini & Laffitte 1949

t/°C	P/Pa
0	5906
5	7693
10	9932
15	12679
20	16092
25	20093
30	24891
35	31651
40	37530
45	45329
50	54382
55	64821
60	76727

Cidlinsky & Polak 1969
in Boublik et al. 1984

t/°C	P/Pa
23.5	18654
25.29	20194
27.42	22177
32	26963
34.22	29591
36.93	32980
41.17	39005
44.08	43639
46.7	48085
48.57	51514
50.96	56204
54.52	63829
56.12	67372
58.17	72427
60.68	78891
63.21	89995
64.66	89995
65.75	93316
67.21	97.734
bp/°C	68.339
eq. 2	P/kPa
A	5.97081
B	1137.408
C	218.516

Ambrose et al. 1976
comparative ebulliometry

t/°C	P/Pa
11.629	10662
15.253	12712
18.945	15122
22.489	17778
27.115	21812
31.087	25839
35.626	31160
40.08	37199
44.778	44561
49.953	53861
54.454	63367
59.24	74743
64.423	88818
68.397	100951
69.209	103576
73.855	119720
78.057	135878
83.078	157382
87.857	180219
91.972	201847
25	19880
Antoine	
eq. 2	P/kPa
A	5.97678
B	1143.073
C	–53.810
bp/K	341.66

coefficients of Chebyshev also given in text.

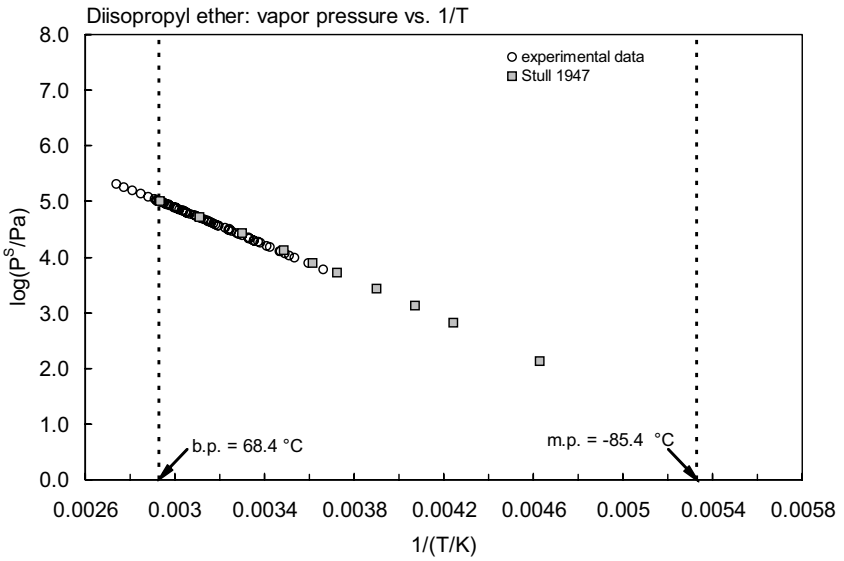
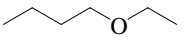


FIGURE 10.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for di-isopropyl ether.

10.1.1.6 Butyl ethyl ether



Common Name: Butyl ethyl ether
Synonym: butyl ethyl ether, 1-ethoxybutane, *n*-butylethyl ether, 3-oxaheptane
Chemical Name: butylethyl ether, 1-ethoxybutane, *n*-butylethyl ether
CAS Registry No: 628-81-9
Molecular Formula: $C_6H_{14}O$, $C_4H_9OCH_2CH_3$
Molecular Weight: 102.174
Melting Point (°C):
–124 (Lide 2003)
Boiling Point (°C):
92.3 (Lide 2003)
Density (g/cm^3 at 20°C):
0.7495, 0.7448 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
136.3 (20°C, calculated-density)
150.5 (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. Additional data at other temperatures designated * are compiled at the end of this section):
6500* (20°C, shake flask-GC/TC, measured range 0–90.7°C, Stephenson 1992)

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):
303164* (126.67°C, static-Bourdon gauge, measured range 126.67–237.78°C, Kobe et al. 1956)
13912* (38.18°C, ebulliometry, measured range 38.18–91.38°C, Cidlinsky & Polak 1969; quoted, Boublik et al. 1984)
log (P/kPa) = 6.06257 – 1252.485/{(T/K) + 56.685} (Antoine eq., Ambrose et al. 1976)
9090 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.06565 – 1234.258/(226.668 + t/°C); temp range 38.18–91.38°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9444 – 1256.4/(216.9 + t/°C); temp range 38–92°C (Antoine eq., Dean 1985, 1992)
7461 (quoted, Riddick et al. 1986)
log (P/kPa) = 6.06257 – 1252.485/(216.465 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
7510 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.062575 – 1252.485/(–56.685 + T/K); temp range 311–365 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 8.5224 – 2.4667 × 10^3/(T/K) + 1.0513·log (T/K) – 1.4047 × 10^{-2}·(T/K) + 9.2664 × 10^{-6}·(T/K)^2; temp range 170–531 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
136 (calculated-P/C from selected data)
241 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
2.03 (shake flask-GC, Hansch & Anderson 1967)
2.03 (recommended, Sangster 1989)
2.03 (recommended, Hansch et al. 1995)

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

3.89 (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, $t_{½}$:

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:

$k_{OH} = 2.28 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 1.34 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 294 ± 2 K (relative rate, Bennett & Kerr 1989)

$k_{OH} = (13.4 - 22.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 294–298 K (review, Atkinson 1989)

$k_{OH} = (18.7 \pm 0.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K (pulse radiolysis-UV spectroscopy, Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance $t_{½} < 0.24$ h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.6.1
Reported aqueous solubilities of butyl ethyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	S/g·m^{-3}
0	10900
9.3	8300
20	6500
31.2	5300
39.7	5800
50.8	4600
60.2	5100
70.2	3900
80.2	4300
90.7	4000

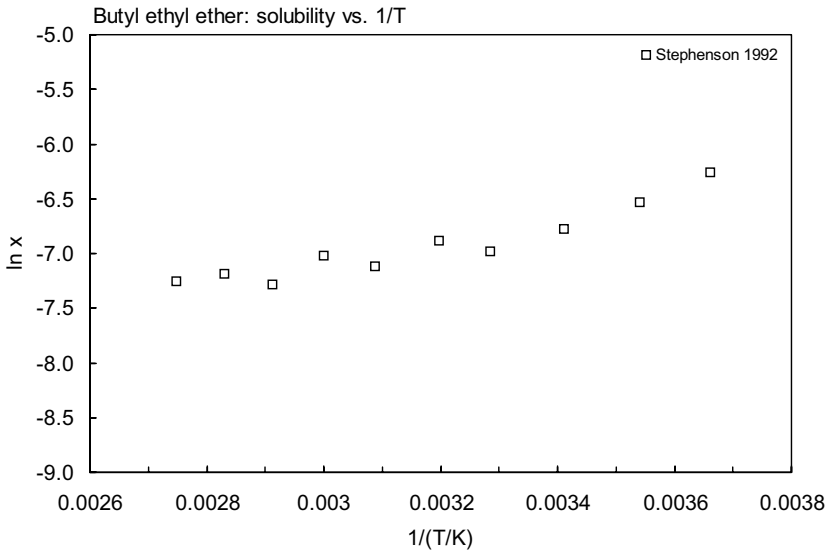


FIGURE 10.1.1.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for butyl ethyl ether.

TABLE 10.1.1.6.2
Reported vapor pressures of butyl ethyl ether 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)		

Kobe et al. 1956				Cidlinsky & Polak 1969			
static-Bourdon gauge				in Boublik et al. 1984			
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
126.67	303164	204.44	1329789	38.18	13912	79.64	67966
132.22	344505	210	1453811	42.31	16695	82.25	74080
137.78	385846	215.56	1591613	44	17950	85.08	81073
143.33	434076	221.11	1736305	49.04	22146	86.71	85441
148.89	489197	226.67	1894778	52.27	25259	89.73	92885
154.44	544318	232.22	2959149	55.1	28420	91.38	98581
160	613219	237.78	2232392	58.73	32451		
165.56	675230			61.25	35696	bp/°C	92.267
171.11	744131			63.22	38339	Antoine	
176.67	826812			65.85	42271	eq. 2	P/kPa
182.22	909493			68.51	46517	A	6.06565
187.78	1005955			71.66	51925	B	1254.258
193.33	1102416			73.74	55807	C	216.668
198.89	1212658			77.12	62513		

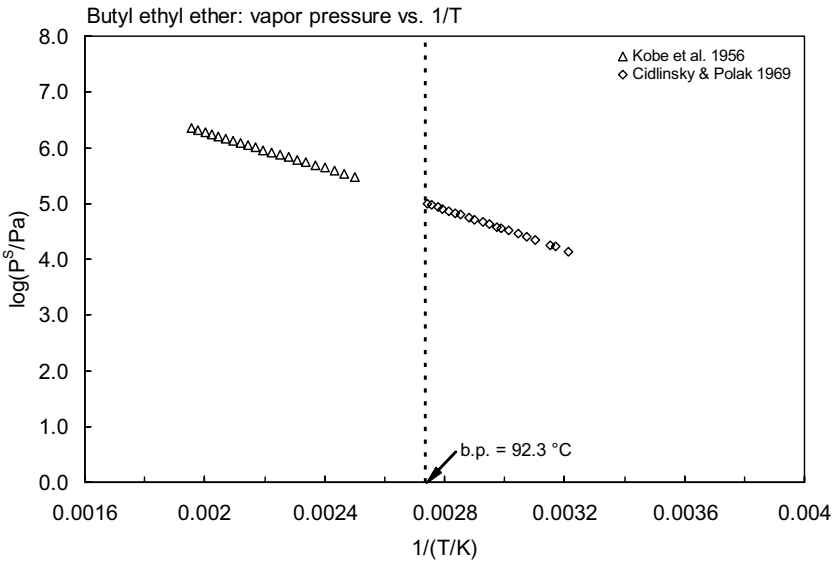
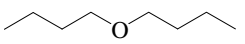


FIGURE 10.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for butyl ethyl ether.

10.1.1.7 Di-*n*-butyl ether



Common Name: Di-*n*-butyl ether
Synonym: 1-butoxybutane, butyl ether, dibutyl ether, *n*-butyl ether, 5-oxanonane, 1,1′-oxybisbutane
Chemical Name: butyl ether, dibutyl ether, di-*n*-butyl ether, *n*-butyl ether, 5-oxanonane, 1,1′-oxybisbutane
CAS Registry No: 142-96-1
Molecular Formula: $C_8H_{18}O$, $(n\text{-}C_4H_9)_2O$
Molecular Weight: 130.228
Melting Point (°C):
–95.2 (Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
140.28 (Lide 2003)
Density (g/cm^3 at 20°C):
0.76889, 0.76461 (20°C, 25°C, Dreisbach & Martin 1949)
0.7684. 0.7641 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
170.0 (calculated-density, Wang et al. 1992)
196.0 (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: 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):
< 100 (17°C, synthetic method, Bennett & Phillip 1928)
300 (20°C, Verschueren 1983; Riddick et al. 1986)
230* (19.9°C, shake flask-GC/TC, measured range 0–90.6°C, Stephenson 1992)

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):
7605* (66.84°C, ebulliometry, measured range 67–142°C, Dreisbach & Shrader 1949)
log (P/mmHg) = 7.31540 – 1648.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
80612* (237.78°C, static method-Bourdon gauge, measured range 238–293°C, Kobe et al. 1956)
19529* (89.14°C, ebulliometry, measured range 89.14–140°C, Cidlinsky & Polak 1969)
log (P/kPa) = 5.93018 – 1302.768/(T/K– 81/481); temp range 89–140°C (Cidlinsky & Polak 1969)
log (P/kPa) = 5.93018 – 1302.768/{(T/K) – 81.481} (Antoine eq., ebulliometry, Ambrose et al. 1976)
640 (20°C, Verschueren 1983)
825, 874 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.151 – 1458.718/(141.982 + t/°C); temp range 66.8–141.97°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 5.92274 – 1298.256/(191.144 + t/°C); temp range 89.14–140.06°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.7963 – 1297.3/(191.03 + t/°C); temp range 89–140°C (Antoine eq., Dean 1985, 1992)
898 (select, Riddick et al. 1986)
log (P/kPa) = 5.930185 – 1302.768/(191.669 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
log (P_L/kPa) = 6.4403 – 1648.4/(–42.15 + T/K); temp range 339–415 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.0537 – 1398.8/(–69.55 + T/K); temp range 336–415 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = $12.9321 - 3.0416 \times 10^3/(T/K) + 0.42929 \cdot \log (T/K) - 1.237 \times 10^{-2} \cdot (T/K) + 7.5943 \times 10^{-6} \cdot (T/K)^2$; temp range 178–581 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

608.5 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
350, 1362 (calculated-group contribution calculated-bond contribution, Hine & Mookerjee 1975)

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

3.08 (calculated-f const., Hansch & Leo 1979)
3.21 (shake flask-GC, Funasaki et al. 1984)
3.21 (recommended, Sangster 1989)
3.21 (recommended, Hansch et al. 1995)

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

3.89 (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, $t_{½}$:

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:
$k_{OH} = (27.8 \pm 3.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)
$k_{OH} = 17 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 294 ± 2 K (relative rate method, Bennett & Kerr 1989)
$k_{OH} = (17.0 - 27.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 294–298 K (review, Atkinson 1989)
$k_{OH} = (27.2 \pm 0.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by pulse radiolysis-UV spectroscopy; $k_{OH} = (28.8 \pm 1.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.7.1
Reported aqueous solubilities of di-*n*-butyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	S/g·m^{-3}
0	400
9.3	320
19.9	230
30.9	230
40.3	200
50.3	220
61.3	120
70.5	150
80.7	90
90.5	100

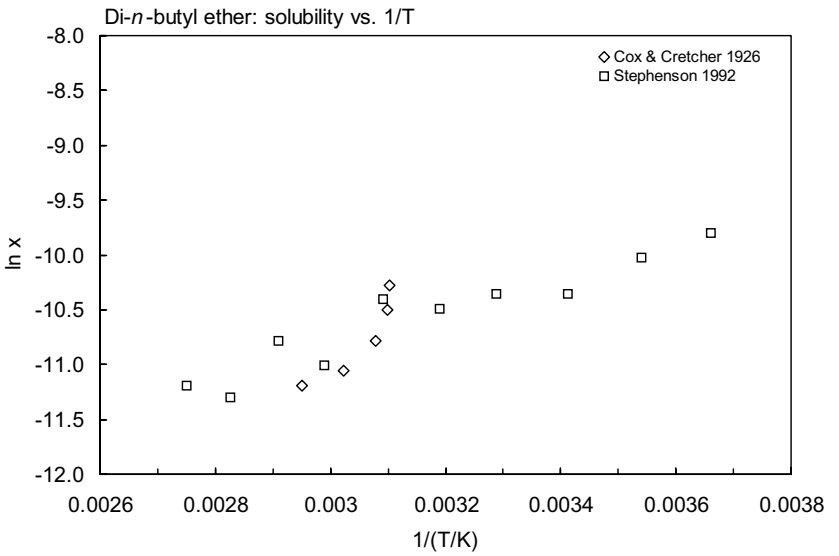


FIGURE 10.1.1.7.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for di-*n*-butyl ether.

TABLE 10.1.1.7.2
Reported vapor pressures of di-*n*-butyl ether 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·log (T/K)	(4)		

Dreisbach & Shrader 1949		**Kobe et al. 1956**		**Cidlinsky & Polak 1969**			
ebulliometry		**static method-Bourdon gauge**		**in Boublik et al. 1984**			
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
66.84	7605	237.78	806142	89.14	19529	129.67	75155
73.6	10114	243.33	895713	94.57	23957	132.04	80429
85.75	16500	248.89	978394	106.43	36288	134.24	85661
112.28	42066	254.44	1061075	110.54	41580	136.13	90298
127.73	67661	260	1143757	113.28	45509	137.72	94456
141.97	101325	265.56	1247108	114.85	47781	140.06	100666
		271.11	1357350	118.2	53253		
		276.67	1474481	121.05	58118	bp/°C	140.295
		282.22	1598503	123.18	62051	eq. 2	P/kPa
		287.78	1729415	123.41	62509	A	5.92274
		293.33	1874107	125.27	66052	B	1298.256
				127.67	70427	C	191.144

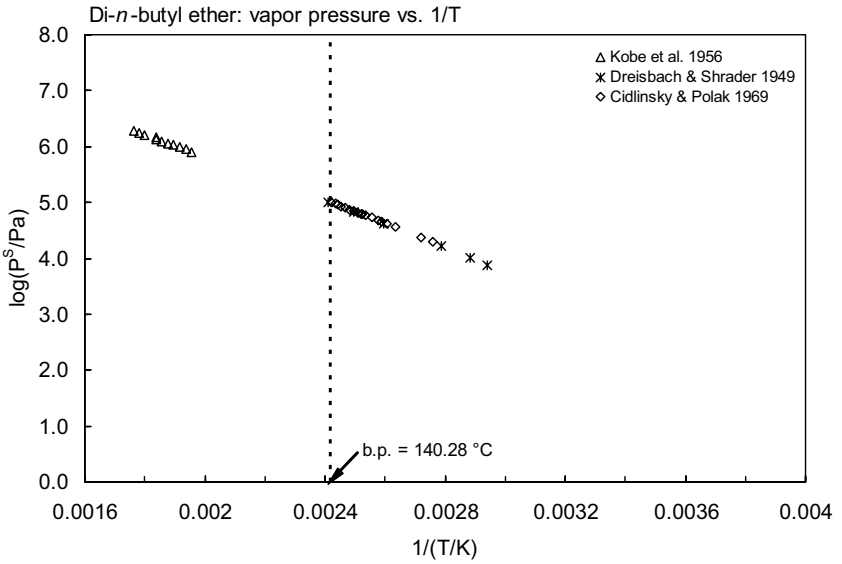


FIGURE 10.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-butyl ether.

10.1.1.8 1,2-Propylene oxide

Common Name: 1,2-Propylene oxide
Synonym: 1,2-epoxypropane, methyloxirane, propylene oxide
Chemical Name: 1,2-propylene oxide, 1,2-epoxypropane, propylene oxide
CAS Registry No: 75-56-9
Molecular Formula: C_3H_6O
Molecular Weight: 58.079
Melting Point (°C):
–111.9 (Lide 2003)
Boiling Point (°C):
35 (Lide 2003)
Density (g/cm^3 at 20°C):
0.859 (0°C, Verschueren 1983)
Molar Volume (cm^3/mol):
69.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
6.57, 6.53 (exptl., Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
476000 (US EPA 1981; quoted, Howard 1989)
405000, 650000 (20°C, 30°C, Verschueren 1983)
259000 (literature data compilation, Yaws et al. 1990)
139320 (calculated-group contribution method,Kühne et al. 1995)

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):
74520* (calculated-Antoine eq. regression, temp range –75 to 34.5°C, Stull 1947)
530538* (87.78°C, static method, measured range 88–204°C, Kobe et al. 1956)
51969* (17.05°C, ebulliometry, measured range –24.17 to 34.75°C (McDonald et al. 1959)
log (P/mmHg) = 6.96997 – 1065.27/(226.283 + t/°C); temp range –24.17 to 34.75°C (ebulliometry, McDonald et al. 1959)
70112* (interpolated-Antoine eq., static method, measured range 19.0–71.8°C Bott & Sadler 1966)
log (P/mmHg) = 7.658 – 1472/(T/K); temp range 19.0–71.8°C (Antoine eq., static method, Bott & Sadler 1966)
log (P/mmHg) = [–0.2185 × 7295.8/(T/K)] + 8.093473; temp range –75 to 34.5°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = 7.06492 – 1113.6/(232.0 + t/°C); temp range –35 to 130°C (Antoine eq., Dean 1985, 1992)
59300, 75900 (20, 25°C, Riddick et al. 1986)
log (P/kPa) = 6.09487 – 1065.27/(226.283 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
71700 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.09487 – 1065.27/(–46.867 + T/K); temp range 225–308 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 38.5381 – 2.631 × 10^3/(T/K) – 11.104·log (T/K) + 4.2178 × 10^{-10}·(T/K) + 5.5025 × 10^{-6}·(T/K)^2; temp range 161–482 K (vapor pressure eq., Yaws 1994)
log (P/kPa) = 6.14068 – 1086.37/[(T/K) – 44.556]; temp range not specified (Antoine eq., Horstmann et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C):
8.653 (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, log K_{OW}:
0.03 (shake flask, Hansch & Leo 1985, 1987)

0.03 (recommended, Sangster 1989)
0.03 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

–0.20, –0.40 (calculated, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:

0.623 (estimated-S, Lyman et al. 1982; quoted, Howard 1989)
1.477 (calculated-QSAR, Sabljic 1984; quoted, Howard 1989)

Environmental Fate Rate Constants, k, and Half-Lives,:

Volatilization: $t_{½}$(calc) ~ 3 and 18 d from a representative or natural river and oligotrophic lake, respectively (USEPA 1986; 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}(exptl) = 5.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 4.5×10^{-13} cm^3 $molecule^{-1}$ s^{-1} for gas phase reactions; k = 2.4×10^8 cm^3 mol^{-1} s^{-1} for the reaction with photochemically produced OH radical in water at room temp. (Güesten et al. 1981; quoted, Howard 1989)

photooxidation $t_{½}$ = 19.3 d can be calculated for the gas phase reaction with OH radical in air by using Güesten 1981 data and assuming an average OH radical concn. of 8×10^5 molecules/cm^3 (GEMS 1986; quoted, Howard 1989)

k_{OH} = $(1.11 \pm 0.75) \times 10^{-12}$ cm^3 $molecule^{-1} \cdot s^{-1}$ with reference to *n*-butane for the gas phase reaction with OH radical in air at (23.1 ± 1.1)°C with an atmospheric lifetime of 10 d for an average concentration of 1×10^6 molecules/cm^3 of OH radical (Edney et al. 1986)

k_{OH}(calc) = 5.4×10^{-13} cm^3 $molecule^{-1}$ s^{-1}; k_{OH}(exptl) = 5.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

k_{OH} = $(4.95 \pm 0.52) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

k_{OH} = 4.95×10^{-13} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 4.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

Hydrolysis: estimated $t_{½}$ ~ 11.6 d in fresh water at pH 7 to 9 and $t_{½}$ = 6.6 d at pH 5 (Howard 1989).

Biodegradation:

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 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

atmospheric lifetime of 10 d (Edney et al. 1986);

$t_{½}$ = 19.3 d, based on estimated photooxidation half-life in air by using Güesten et al. 1981 data and assuming an average OH radical concn. of 8×10^5 molecules/cm^3 (GEMS 1986; quoted, Howard 1989).

Surface water: calculated $t_{½}$ = 9.15 yr in natural water by using Güesten et al. 1981 data and assuming an average OH radical concentration of 1×10^{-17} M in natural water (Howard 1989).

Ground water:

Sediment:

Soil:

Biota:

TABLE 10.1.1.8.1
Reported vapor pressures of 1,2-propylene oxide 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·log (T/K)	(4)		

Stull 1947		Kobe et al. 1956		McDonald et al. 1959		Bott & Sadler 1966	
summary of lit. data		static-Bourdon gauge		ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–75.0	133	87.78	530538	–24.7	6665	19	55462
–57.8	666.6	93.33	599439	–13.66	12170	27	76527
–49.0	1333	98.89	675230	0.77	25345	36.3	107457
–39.8	2666	104.44	771691	17.05	51969	40.8	126656
–28.4	5333	110	868153	33.11	97379	46.8	154253
–21.3	7999	115.56	978394	34.75	103298	50.2	168652
–12.0	13332	121.11	1102416			54	193583
2.1	26664	126.67	1226438			59.2	225847
17.8	53329	132.22	1378020	eq. 2	P/mmHg	64.7	265844
34.5	101325	137.78	1536492	A	6.96997	71.8	320373
		143.33	1701855	B	1065.27		
mp/°C	–112.1	148.89	1880997	C	233.386	eq. 1	P/mmHg
		154.44	2073920			A	7.658
		160	2273733	mp/°C	–112.13	B	1472
		165.56	2506996				
		171.11	2762930				
		176.67	3017864				
		182.22	3300358				
		187.78	3589742				
		193.33	3906687				
		198.89	4251192				
		204.44	4602587				

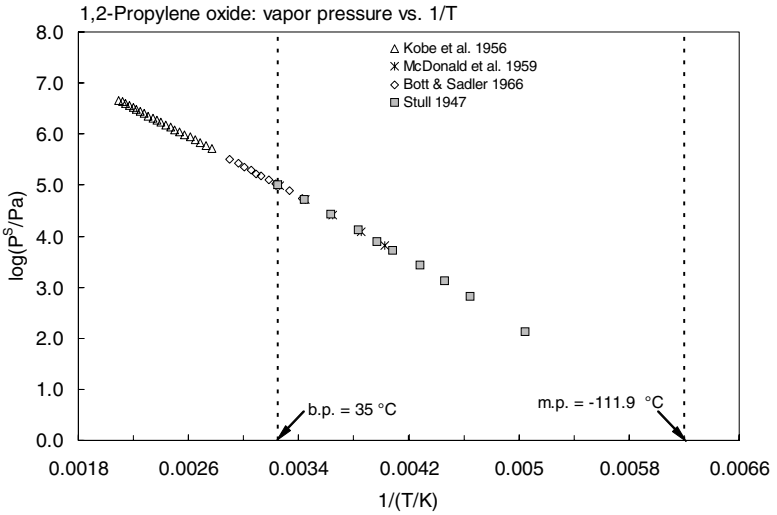


FIGURE 10.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2-propylene oxide.

10.1.1.9 Furan

Common Name: Furan
Synonym: 1,4-epoxy-1,3-butadiene, divinylene oxide, furfuran, oxole, tetrole
Chemical Name: 1,4-epoxy-1,3-butadiene, divinylene oxide, furan
CAS Registry No: 110-00-9
Molecular Formula: C_4H_4O
Molecular Weight: 68.074
Melting Point (°C):
–85.61 (Lide 2003)
Boiling Point (°C):
31.5 (Lide 2003)
Density (g/cm^3 at 20°C):
0.9378 (Dreisbach 1955; Riddick et al. 1986)
0.9514 (Weast 1982–83)
Molar Volume (cm^3/mol):
72.6 (20°C, calculated-density)
73.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
3.803 (Riddick et al. 1986)
2.05, 3.80 (exptl., Chickos et al. 1999)
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):
10070 (literature average, Valvani et al. 1981)
10000 (Verschueren 1983)
10000 (Riddick et al. 1986)
9900 (literature data compilation, Yaws et al. 1990)
26500 (calculated-group contribution method, Kühne et al. 1995)

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):
70109* (21.614°C, comparative ebulliometry, measured range 2,552–61.43°C, Guthrie et al. 1952)
log (P/mmHg) = 6.97523 – 1060.851/(t/°C + 227.740); temp range 2.5–61.43°C (Antoine eq., comparative ebulliometry, Guthrie et al. 1952)
79980 (calculated from determined data, Dreisbach 1955)
log (P/mmHg) = 6.97523 – 1060.851/(227.740 + t/°C); temp range –35 to 90°C (Antoine eq. for liquid state, Dreisbach 1955)
627000* (93.33°C, static-Bourdon gauge, measured range 93.33–210°C, Kobe et al. 1956)
log (P/mmHg) = [1– 304.367/(T/K)] × 10^{0.858337 – 8.56435 × 10^{-4}·(T/K) + 9.32123 × 10^{-7}·(T/K)^2}; temp range 340.95–463.65 K (Cox eq., Chao et al. 1983)
70110 (21.61°C, quoted, Boublik et al. 1984)
79930 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.10017 – 1060.871/(227.742 + t/°C); temp range: 2.552–61.43°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.97527 – 1060.87/(227.74 + t/°C); temp range: 2–61°C (Antoine eq., Dean 1985, 1992)
84530 (selected, Riddick et al. 1986)
log (P/kPa) = 6.10013 – 1060.851/(227.74 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
79930 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.10013 – 1060.851/(–45.41 + T/K); temp range 238–363 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 24.9555 – 2.1624×10^3/(T/K) –6.1066·log (T/K) – 2.4185×10^{-10}·(T/K) + 2.0858×10^{-6}·$(T/K)^2$; temp range 188–490 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

575.5 (calculated-P/C using Riddick et al. 1986 data)
545.8 (computed-vapor liquid equilibrium (VLE) data, Yaws et al. 1991)

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

1.34 (Hansch & Leo 1979;)
1.13 (estimated-HPLC, Garst 1984)
1.14, 1.35 (estimated-MO, π substituent consts., Bodor et al. 1989)
1.34 (recommended, Sangster 1989)
1.34 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.50, 1.46; 1.48 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

Environmental Fate Rate Constant, 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:

$k = 1.4 \times 10^8$ M^{-1} s^{-1} oxidation rate by singlet oxygen in water (Mill 1980; quoted, Mill & Mabey 1985)
$k_{OH} = (4.01 \pm 0.30) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} with a atmospheric lifetime τ ~ 7 h, $k_{O3} = (2.42 \pm 0.28) \times 10^{-18}$ cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K; and $k_{O(3P)} \sim 1.0 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} for the reaction with $O(^3P)$ atom at 298 K (relative rate method, Atkinson et al. 1983)
$k_{OH} = (3.98 \pm 0.35) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 22 ± 2°C (relative rate method, Tuazon et al. 1984)
$k_{OH}^* = (40.8, 43.1) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 297 K, measured range 254–424 K (FP-RF flash photolysis-resonance fluorescence, Wine & Thompson 1984)
$k_{O3} = 2.4 \times 10^{-18}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 0.15 d^{-1}, $k_{OH} = 4.0 \times 10^{-1}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 3.5 d^{-1}, and $k_{NO3} = 1.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 29 d^{-1} at room temp. (review, Atkinson & Carter 1984)
$k_{O3} = 2.4 \times 10^{-18}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 0.15 d^{-1}, $k_{OH} = 4.0 \times 10^{-1}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 1.7 d^{-1}, and $k_{NO3} = 1.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 29 d^{-1} at room temp. (review, Atkinson 1985)
$k_{NO3} = (1.4 \pm 0.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 ± 2 K (relative rate method, Atkinson et al. 1985)
$k_{O3} = 2.4 \times 10^{-18}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime τ = 6.7 d, $k_{OH} = 4.0 \times 10^{-1}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated τ = 6.9 h, and $k_{NO3} = 1.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated τ = 50 min at room temp. (Atkinson et al. 1985)
$k_{OH} = 4.07 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} (Atkinson 1987,1988; quoted, Müller & Klein 1991)
$k_{OH} = 4.046 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, $k_{NO3} = 1.439 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (Atkinson 1986 and Atkinson et al. 1988, Sabljic & Güsten 1990; Atkinson 1991)
$k_{NO3} = 1.44 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (relative rate method, Atkinson et al. 1988, Atkinson 1991)
$k_{OH}^* = 4.05 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

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

Half-Lives in the Environment:

Air: disappearance $t_{½} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
calculated atmospheric lifetimes: 6.7 d due to reaction with O_3 in 24-h, 6.9 h due to reaction with OH radical in daytime and 50 min with NO_3 radical at room temp. (Atkinson et al. 1985).

Surface water: $t_{½} = 1.0$ h, estimated from oxidation rate by singlet oxygen of 1.4×10^8 M^{-1} s^{-1} (Mill 1980; quoted, Mill & Mabey 1985).

Ground water:

Sediment:

Soil:

Biota:

TABLE 10.1.1.9.1
Reported vapor pressures of furan 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)		

Guthrie et al. 1952				**Kobe et al. 1956**			
comparative ebulliometry				**static-Bourdon gauge**			
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
2.552	31160	56.329	232087	93.33	627000	154.44	2156601
7.267	38547	61.43	270110	98.89	709680	160	2370194
12.018	47359			104.44	806142	165.56	1597568
16.797	57803	bp/°C	31.36	110	909493	171.11	2838721
21.614	70109	ΔH_V/(kJ mol^{-1}) =	27.09	115.56	1019735	176.67	3107435
26.469	84525		at bp	121.11	1150647	182.22	3389929
31.357	101325			126.67	1295339	187.78	3686204
36.279	120790	eq. 2	P/mmHg	132.22	1440031	193.33	3996258
41.241	143268	A	6.97523	137.78	1605393	198.89	4326983
46.232	169052	B	1060.851	143.33	1770756	204.44	4671488
51.265	198530	C	227.74	149.89	1956788	210	5009103

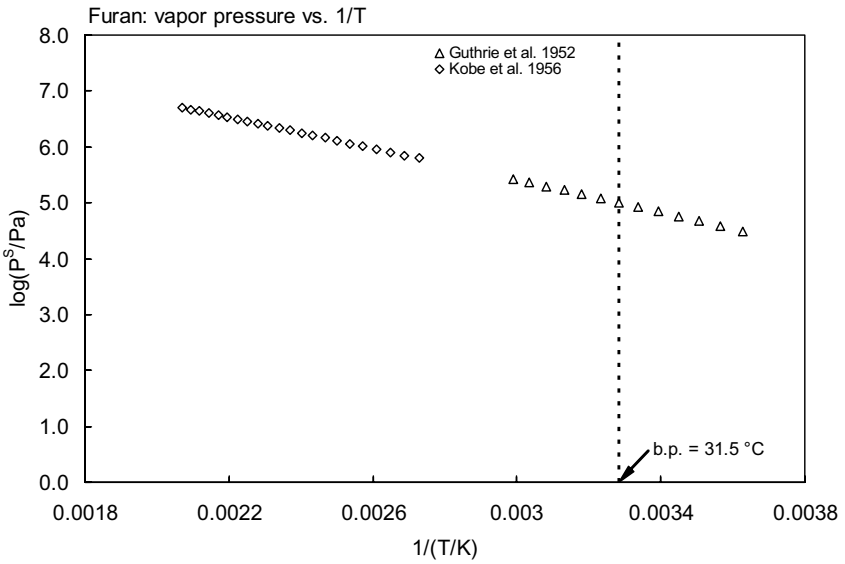


FIGURE 10.1.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for furan.

10.1.1.10 2-Methylfuran

Common Name: 2-Methylfuran
Synonym: silvan, sylvan
Chemical Name: 2-methylfuran
CAS Registry No: 534-22-5
Molecular Formula: C_5H_6O
Molecular Weight: 82.101
Melting Point (°C):
–91.3 (Lide 2003)
Boiling Point (°C):
64.7 (Lide 2003)
Density (g/cm^3 at 20°C):
0.913 (Verschueren 1983)
Molar Volume (cm^3/mol):
89.9 (20°C, calculated-density)
95.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
8.66 (exptl., Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
3000 (20°C, Verschueren 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):
358285* (110°C, static-Bourdon gauge, measured range 110–254.44°C, Kobe et al. 1956)
86126* (60.3°C, isoteniscope/manometry, measured range 60.3–100.3°C, Eon et al. 1971)
log (P/mmHg) = [1– 338.704/(T/K)] × 10^{0.871223 – 7.95690 × 10^{-4}·(T/K) + 7.81737 × 10^{-7}·$(T/K)^2$}; temp range 333.45–527.61 K (Cox eq., Chao et al. 1983)
18930, 29990 (20°C, 30°C, quoted, Verschueren 1983)
23090 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.81244 – 1641.052/(276.164 + t/°C); temp range 60.3–100.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
23250 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.95585 – 1107.3/(–56.88 + T/K); temp range 251–338 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
518 (20°C, calculated-P/C using Verschueren 1983 data)

Octanol/Water Partition Coefficient, log K_{OW}:
1.85 (shake flask, Log P Database, Hansch & Leo 1987)
1.85 (recommended, Sangster 1989)
1.85 (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 $t_{½} < 0.24$ h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.1.10.1
Reported vapor pressures of 2-methylfuran 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)		

Kobe et al. 1956				Eon et al. 1971			
static-Bourdon gauge				isoteniscope/manometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
110	358285	160	1088636	210	2521777	60.3	86126
115.56	413406	165.56	1205768	215.56	2749150	70.3	119057
121.11	468527	171.11	1329789	221.11	2990303	80.3	161720
126.67	537428	176.67	1467591	226.67	3231457	90.3	215982
132.22	606329	182.22	1612283	232.22	3493281	100.3	283977
137.78	689010	187.78	1770756	237.78	3768885		
143.33	778581	193.33	1943008	243.33	4065159		
149.89	888823	198.89	2122151	248.89	4382104	ΔH_V/(kJ mol^{-1}) = 30.79	
154.44	978394	204.44	2321964	254.44	4719719		

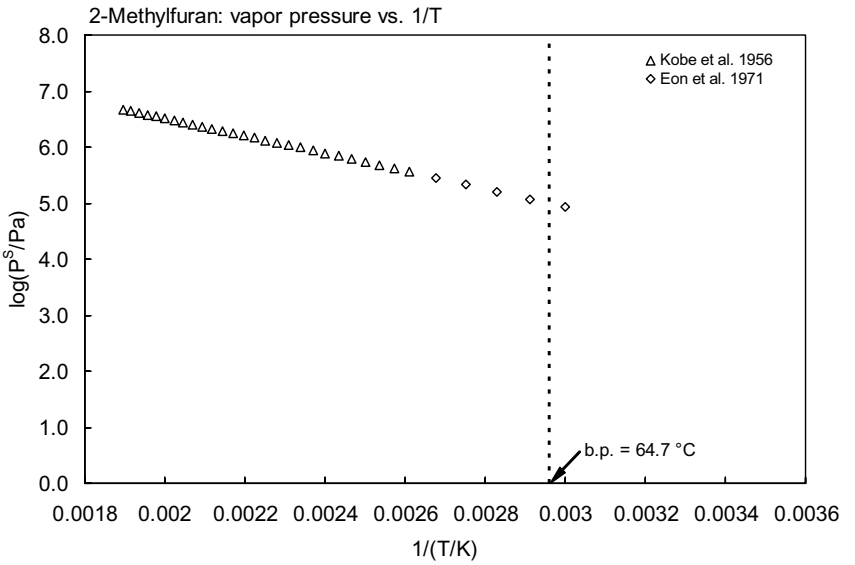


FIGURE 10.1.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for methylfuran.

10.1.1.11 Tetrahydrofuran

Common Name: Tetrahydrofuran
Synonym: 1,4-epoxybutane, diethylene oxide, oxacyclopentane, tetramethylene oxide
Chemical Name: 1,4-epoxybutane, diethylene oxide, oxacyclopentane, tetrahydrofuran, tetramethylene oxide
CAS Registry No: 109-99-9
Molecular Formula: C_4H_8O
Molecular Weight: 72.106
Melting Point (°C):
–108.44 (Lide 2003)
Boiling Point (°C):
65 (Lide 2003)
Density (g/cm^3 at 20°C):
0.8880 (Verschueren 1983)
0.8892 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
81.1 (20°C, calculated-density)
88.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
8.535 (quoted, Riddick et al. 1986)
8.54 (exptl., Chickos et al. 1999)
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):
miscible (Verschueren 1983; 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):
23465* (dynamic-ebulliometry, measured 15–65°C, Flom et al. 1951)
434076* (121.11°C, static-Bourdon gauge, measured range 121.11–265.56°C, Kobe et al. 1956)
19920* (23.139°C, measured range 23.2–99.7°C, Scott et al. 1970)
21646* (measured range 0.35–35°C, Koizumi & Ouchi 1970; quoted, Boublik et al. 1984)
log (P/mmHg) = [1– 339.244/(T/K)] × 10^{0.830424 – 6.81525 × 10^{-4}·(T/K) + 6.84786 × 10^{-7}·(T/K)^2}; temp range 253.15–540.15 K (Cox eq., Chao et al. 1983)
17530, 26340 (20°C, 30°C, quoted, Verschueren 1983)
21610, 21630 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.59372 – 1446.15/(249.982 + t/°C); temp range 0.35–35°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.12023 – 1202.394/(226.267 + t/°C); temp range 23.139–99.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.97231 – 540.5/(260.10 + t/°C); temp range not specified (Antoine eq., Dean 1985, 1992)
19920, 21600, 26870 (23.139, 25, 30°C, Riddick et al. 1986)
log (P/kPa) = 6.79696 – 1157.06/(t/°C + 206.75), temp range: 90–140°C, (Antoine eq., Riddick et al. 1986)
21620, 21900 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.92617 – 1101.47/(–57/95 + T/K); temp range 273–339 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.12052 – 1202.561/(–46.863 + T/K); temp range 296–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.63507 – 1626.656/(15.041 + T/K); temp range 399–479 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.73137 – 1702.922/(23.613 + T/K); temp range 467–541 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/mmHg) = $34.870 - 2.7523 \times 10^3/(T/K) - 9.5958 \cdot \log (T/K) + 1.9889 \times 10^{-10} \cdot (T/K) + 3.5465 \times 10^{-6} \cdot (T/K)^2$; temp range 165–540 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

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

10.33, 142.6 (calculated-group contribution calculated-bond contribution method, Hine & Mookerjee 1975)

Octanol Water Partition Coefficient, log K_{OW}:

0.46 (calculated-f const., Hansch & Leo 1979)

0.22 (shake flask-GC, Funasaki et al. 1985)

0.46 (shake flask, Log P Database, Hansch & Leo 1987)

0.46 (recommended, Sangster 1989)

0.46 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.37, 1.26; 1.33 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 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:

$k_{OH} = (1.59 - 1.63) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (FP-RF flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)

k_{OH}(calc) = 1.66×10^{-11} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.5×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH}(exptl) = 1.50×10^{-11} $cm^3 \cdot molecule^{-1}$ s^{-1}, k_{OH}(calc) = 1.28×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1986, 1987; quoted, Sabljic & Güsten 1990)

k_{OH}(calc) = 1.28×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987, 1988; quoted, Müller & Klein 1991)

$k_{NO3} = 4.875 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Atkinson 1991)

$k_{NO3} = 4.88 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (relative rate method, Atkinson et al. 1988, Atkinson 1991)

$k_{OH} = 1.78 \times 10^{-11}$ $cm^3 \cdot molecule^{-1}$ s^{-1} at 296 K (RP-RF method, Wallington et al. 1988b)

$k_{OH} = 1.61 \times 10^{-11}$ $cm^3 \cdot molecule^{-1}$ s^{-1} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH}* = 18.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1} by relative rate method; $k_{OH} = 16.7 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 16 h at 298 ± 2 K; measured range 263–372 K (Moriarty et al. 2003)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance $t_{½} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water:

Ground water:

Sediment:
Soil: disappearance $t_{½}$ = 5.7 d was calculated from measured first-order rate constant (Anderson et al. 1991).
Biota:

TABLE 10.1.1.11.1
Reported vapor pressures of tetrahydrofuran 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)		

Flom et al. 1951		**Kobe et al. 1956**		**Koizumi & Ouchi 1970**		**Scott 1970**	
dynamic-ebulliometry		**static-Bourdon gauge**		**in Boublik et al. 1984**		**comparative ebulliometry**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
15	15199	121.11	434076	0.35	567	23.139	19920
25	23465	126.67	509867	10	10732	28.362	25007
35	35064	132.22	578768	15	13687	33.62	31160
45	51329	137.78	661450	20	17240	38.917	38547
55	73327	143.33	744131	25	21646	44.251	47359
65	101325	148.89	833702	30	26842	49.62	57803
		154.44	909493	35	35031	55.029	70109
bp/°C	66.1	160	1005955			60.475	84525
		165.56	1116196			65.965	101325
		171.11	1233328			71.489	120.789
		176.67	1364240			77.054	143.268
		182.22	1502042			82.659	169052
		187.78	1653624			88.3	198530
		193.33	1777646			93.98	232087
		198.89	1984349			99.7	270110
		204.44	2156601				
		210	2349524			mp/°C	
		215.56	2549337				
		21.11	2769820				
		226.67	3004084				
		232.22	3252127				
		237.78	3507061				
		243.33	3782655				
		248.89	4078939				
		254.44	4388994				
		260	4705938				
		265.56	5050443				

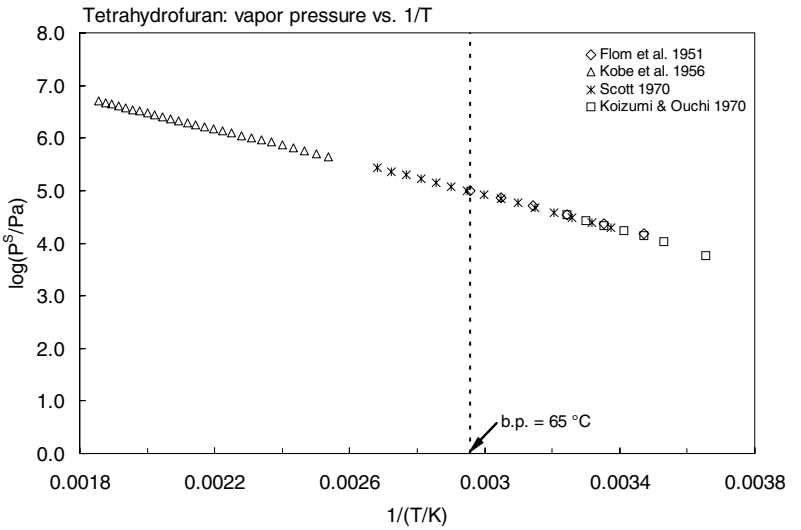


FIGURE 10.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for tetrahydrofuran.

10.1.1.12 Tetrahydropyran

Common Name: Tetrahydropyran
Synonym: pentamethylene oxide, oxacyclohexane
Chemical Name: 1,5-epoxypentane, pentamethylene oxide, oxacyclohexane, tetrahydro-2H-pyran
CAS Registry No: 142-68-7
Molecular Formula: $C_5H_{10}O$
Molecular Weight: 86.132
Melting Point (°C):
–49.1 (Lide 2003)
Boiling Point (°C):
88.0 (Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 20°C):
0.8814, 0.8772 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
97.7 (20°C, calculated-density)
107.0 (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: 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):
80200 (selected, Riddick et al. 1986)
85700*, 68800 (19.9°C, 31°C, shake flask-GC/TC, measured range 0–81.3°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9536 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.01171 – 1249.062/(–49.943 + T/K); temp range 273–362 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
12.71 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
13.94, 215.9 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:
0.64 (shake flask-GC, Funasaki et al. 1985)
0.82 (recommended, Sangster 1989)
1.00 (recommended, Sangster 1993)
0.95 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
3.22 (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, $t_{½}$:
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} ~ 13.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} for the gas-phase reactions with OH radical at 298 K (Atkinson 1989)
k_{OH}* = 11.5×10^{-12} cm^3 $molecule^{-1}$ s^{-1} by relative rate method; k_{OH} = 12.3×10^{-12} cm^3 $molecule^{-1}$ s^{-1} by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 28 h at 298 ± 2 K, measured range 263–372 K (Moriarty et al. 2003).

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance $t_{½}$ < 0.24 h from air for the reaction with OH radical (Darnall et al. 1976); photodecomposition $t_{½}$ = 3.4 h under simulated atmospheric conditions, with NO (Dilling et al. 1976).

TABLE 10.1.1.12.1
Reported aqueous solubilities of tetrahydropyran at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	S/g·m^{-3}
0	12900
9.4	10030
19.9	8670
31	6880
39.6	6040
50.5	5160
60.7	4620
71.3	4500
81.3	4290

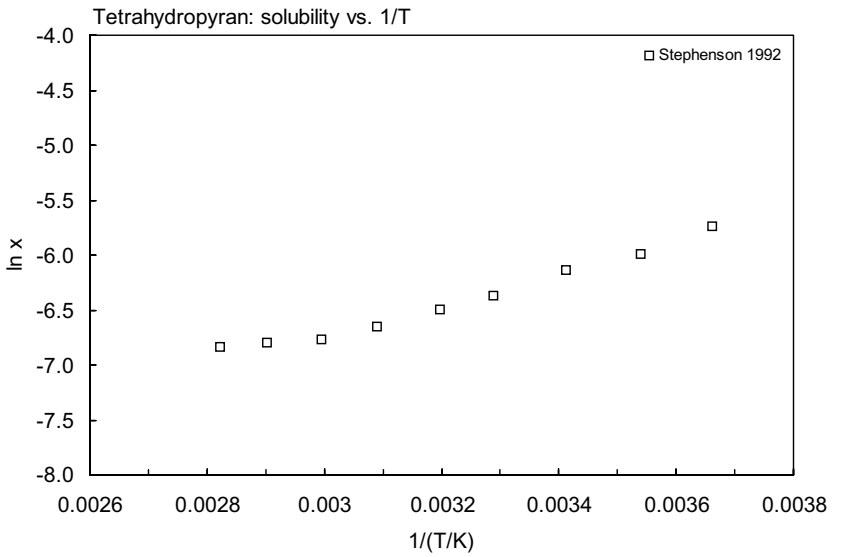


FIGURE 10.1.1.12.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for tetrahydropyran.

10.1.1.13 1,4-Dioxane

Common Name: 1,4-Dioxane
Synonym: 1,4-diethylenedioxide, glycolethyleneether, *p*-dioxane
Chemical Name: 1,4-dioxane
CAS Registry No: 123-91-1
Molecular Formula: $C_4H_8O_2$
Molecular Weight: 88.106
Melting Point (°C):
11.85 (Lide 2003)
Boiling Point (°C):
101.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.03318, 1.02766 (20°C, 25°C, Hovorka et al. 1936)
1.0336, 1.0280 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
85.2 (20°C, calculated-density)
92.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
12.46 (quoted, Riddick et al. 1986)
12.84 (exptl., Chickos et al. 1999)
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):
miscible (Verschueren 1983; Riddick et al. 1986; Howard 1990)
miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations, *data at other temperatures are tabulated at end of this section):
4920* (static method, measured range 10–80°C, Hovorka et al. 1936)
log (P/mmHg) = 8.0588 – 1933.8/(T/K); temp range 10–80°C (Antoine eq., static method, Hovorka et al. 1936)
log (P/mmHg) = 7.8642 – 1866.7/(T/K); temp range ~ 10–110°C (Antoine eq., differential manometer, Gallaugher & Hibbert 1937)
4986* (static-Hg manometer, measured range 20–105°C, Crenshaw et al. 1938; quoted, Vinson & Martin 1963)
log (P/mmHg) = –2316.26/(T/K) – 2.77251·log (T/K) + 16.2007): temp range 20–105°C (Hg manometer, Crenshaw et al. 1938)
5333* (summary of literature data, Stull 1947)
406516* (154.44°C, static-Bourdon gauge, measured range 154.44–310°C, Kobe et al. 1956)
log (P/mmHg) = [–0.2185 × 8546.2/(T/K)] + 7.864110; temp range –35.8 to 101°C (Antoine eq., isomer not specified, Weast 1972–73)
5065 (Boublik et al. 1984)
4932 (quoted, Verschueren 1983)
log (P/kPa) = 6.66014 – 1556.983/(240.366 + t/°C); temp range 20–105°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.56891 – 1550.445/(240.459 + t/°C); temp range 20–125°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
4950, 6135 (25, 30°C, Riddick et al. 1986)
log (P/kPa) = 6.9891 – 1866.7/(T/K), temp range not specified (Antoine eq., Riddick et al. 1986)
4915 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.40318 – 1457.97/(–42.888 + T/K); temp range 285–375 K (Antoine eq., Stephenson & Malanowski 1987)
5060, 6092 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
log (P/mmHg) = 20.5761 – 2.4658×10^3/(T/K) – 4.3645·log (T/K) – 2.7053×10^{-10}·(T/K) + 8.5235×10^{-6} $(T/K)^2$; temp range 285–587 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
0.495 (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975; quoted, Howard 1990)
0.431, 1.564 (calculated-group contribution, calculated-bond contribution method Hine & Mookerjee 1975)
0.698 (computer value, Yaws et al. 1991)
1.609. 4.314, 6.925, 10.19 (dioxane, 40, 60, 70, 80°C, equilibrium headspace-GC, Kolb et al. 1992)
ln ($1/K_{AW}$) = – 7.940 + 4798/(T/K), temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)
0.496 (quoted from Howard 1989–1991, Capel & Larson 1995)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.42, 0.01 (observed, calculated-f const., Chou & Jurs 1979)
–0.42 (quoted, Verschueren 1983; quoted, Pinal et al. 1990)
–0.27 (Hansch & Leo 1985; quoted, Howard 1990; Capel & Larson 1995)
–0.27 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
1.23 (soil, estimated-K_{OW}, Lyman et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization: estimated Henry' law constant suggests that volatilization for 1,4-dioxane from water and moist soil should be slow; however, it has a moderate vapor pressure, so volatilization from dry soil is possible (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 $t_{½}$ = 67 d to 9.1 yr in water, based on measured rates for the reaction with hydroxyl radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; quoted, Howard et al. 1991)
photooxidation $t_{½}$ = 8.1–81 h in air, based on measured rate constant for the reaction of 1,3,5-trioxane with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)
photooxidation $t_{½}$ = 6.69–9.6 h in the atmosphere, based on estimated reaction rate with photochemically produced hydroxyl radicals (Howard 1990)
$k_{OH} = 10.9 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (Atkinson 1989)
k_{OH}(calc) = 38.6×10^{-12} cm^3 mol^{-1} s^{-1}, k_{OH}(exptl) = 10.9×10^{-12} cm^3 mol^{-1} s^{-1} at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)
k_{OH}* = 9.5×10^{-12} cm^3 $molecule^{-1}$ s^{-1} by relative rate method; $k_{OH} = 12.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 25 h at 298 ± 2 K; measured range 263–372 K (Moriarty et al. 2003)
Hydrolysis:
Biodegradation: aqueous aerobic $t_{½}$ = 672–4320 h, based on unacclimated aerobic aqueous screening test data with confirmed resistance to biodegradation (Sasaki 1978; Kawasaki 1980; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 2688–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
$t_{½}$(aerobic) = 28 d, $t_{½}$(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: disappearance $t_{½}$ < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{½}$ = 8.1–81 h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);
$t_{½}$ = 6.69–9.6 h in the atmosphere, based on estimated reaction rate with photochemically produced hydroxyl radical (Howard 1990).

Surface water: $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{½}$ = 1344–8640 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:

TABLE 10.1.1.13.1
Reported vapor pressures of 1,4-dioxane 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)

Hovorka et al. 1936		Crenshaw et al. 1938		Stull 1947		Kobe et al. 1956	
static method		ebulliometry-Hg manometer		summary of literature data		static method-Bourdon gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
10	2266	20	3853	–35.8	133.3	154.44	406516
20	3746	25	4986	–12.8	666.6	160	461637
25	4920	30	6386	–1.20	1333	165.56	523648
30	6346	40	10239	12	2666	171.11	585659
40	10212	50	15905	25.2	5333	176.67	654560
50	15972	60	23985	33.8	7999	182.22	730351
60	24171	70	35224	45.1	13332	187.78	806142
70	35583	80	50503	62.3	26664	193.33	902603
80	51036	90	70821	81.8	53329	198.89	992174
		100	97350	101.1	101325	204.44	1095526
eq. 1	P/mmHg	105	113351			210	1205768
A	8.0588			mp/°C	10	215.56	1322899
B	1933.8	bp/°C	101.26			221.11	1440031
						226.67	1577833
		eq. 4	P/mmHg			232.22	1722525
		A	16.2007			237.78	1874107
		B	2316.26			243.33	2039470
		C	2.77251			248.89	2211722
						254.44	2397755
						260	2597568
						265.56	2797381
						271.11	3052314
						276.67	3259017
						282.22	3507061
						287.78	3755105
						293.33	4037599
						298.89	4333873
						204.44	4595697
						310	4933312

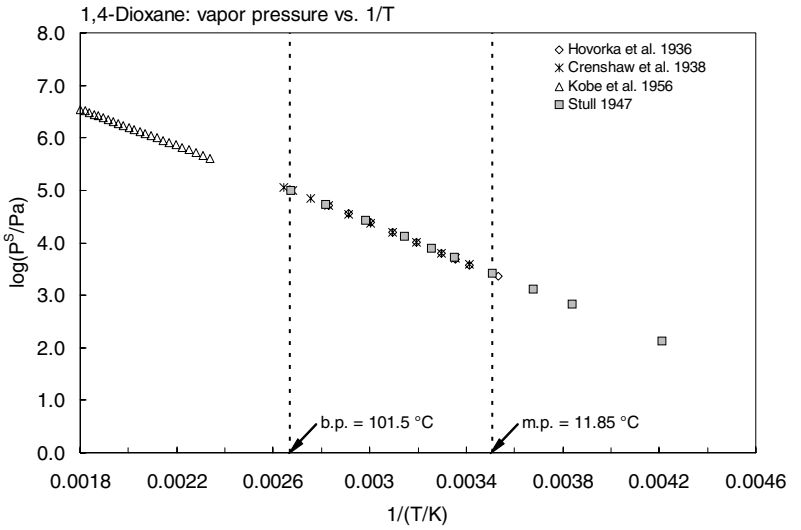
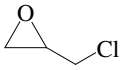


FIGURE 10.1.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for dioxane.

10.1.2 Halogenated ethers

10.1.2.1 Epichlorohydrin



Common Name: Epichlorohydrin
Synonym: 1-chloro-2,3-epoxypropane, (chloromethyl)oxirane, α-epichlorohydrin, γ-chloropropylene oxide
Chemical Name: epichlorohydrin, 1-chloro-2,3-epoxypropane, α-epichlorohydrin, γ-chloropropylene oxide
CAS Registry No: 106-89-8
Molecular Formula: C_3H_5OCl
Molecular Weight: 92.524
Melting Point (°C):
–57.2 (Riddick et al. 1986; Howard 1989)
–26 (Lide 2003)
Boiling Point (°C):
118 (Lide 2003)
Density (g/cm^3 at 20°C):
1.1807, 1.1746 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
78.4 (20°C, calculated-density)
90.9 (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, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
65800 (20°C, selected, Riddick et al. 1986)
65800 (20°C, Krijgsheld & Van der Gen 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2400 (selected, Riddick et al. 1986)
log (P/kPa) = 6.5958 – 1587.9/(230 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
2192 (Daubert & Danner 1985)
log (P_L/kPa) = 6.5958 – 1587.9/(–43.15 + T/K); temp range 328–388 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 24.764 – 2.8846 × 10^3/(T/K) – 5.6252·log (T/K) – 1.1011 × 10^{-10}·(T/K) + 5.3331 × 10^{-7}·(T/K)^2; temp range 216–610 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
3.375 (calculated-P/C using Riddick et al. 1986 data)

Octanol/Water Partition Coefficient, log K_{OW}:
0.30 (Krijgsheld & Van der Gen 1986)
0.45 (shake flask-GC, Deneer et al. 1988)
0.45 (recommended, Sangster 1993)
0.45 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
0.66 (estimated, Santodonato et al. 1980; quoted, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:
2.09 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1989)

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

Volatilization: evaporation $t_{½}$ ~ 29 h for a model river 1 m deep with a 1 m/s current and 3 m/s wind (Lyman 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:

photooxidation $t_{½}$ ~ 4.0 d, based on estimation for the photooxidation with hydroxyl radical in air (Cupitt 1980; quoted, Howard 1989)

k_{OH}(calc) = 9.9×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 4.4×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} \geq 5.5 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} with reference to *n*-butane for the gas phase reaction with OH radical at 23.3 ± 0.9°C with an atmospheric lifetime of < 21 d for an average OH radical concentration of 1×10^6 molecules/cm^3 (Edney et al. 1986)

k_{OH}(exptl) = 4.4×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 6.6×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

k_{O3}(aq.) ≤ 0.003 M^{-1} s^{-1} for direct reaction with ozone in water at pH 4.1 and 22°C, with $t_{½}$ -130 d at pH 7 (Yao & Haag 1991).

Hydrolysis: half-life of 8.2 d in distilled water to hydrolyze to 1-chloropropan-2,3-diol at 20°C and pH 5–9 (Mabey & Mill 1978; quoted, Howard 1989; Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{½}$ = 168–672 h, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Bridie et al. 1979; Sasaki 1978; 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: photodecomposition $t_{½}$ = 16.0 h under simulated atmospheric conditions, with NO (Dilling et al. 1976);

$t_{½}$ ~ 4.0 d, based on estimation for the photooxidation with hydroxyl radical in air (Cupitt 1980; quoted, Howard 1989);

$t_{½}$ = 146–1458 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetime < 21 d due to reactions with OH radical (Edney et al. 1986).

Surface water: evaporation $t_{½}$ = 29 h for a model river 1 m deep with a 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);

$t_{½}$ = 168–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured rate constant k ≤0.003 M^{-1} s^{-1} for direct reaction with ozone in water at pH 4.1 and 22°C, with $t_{½}$ – 130 d at pH 7 (Yao & Haag 1991).

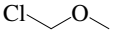
Ground water: 336–1344 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 168–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

10.1.2.2 Chloromethyl methyl ether



Common Name: Chloromethyl methyl ether
Synonym: chloromethyl ether, chloromethoxymethane, CMME, monochlorodimethyl ether
Chemical Name: chloromethyl methyl ether
CAS Registry No: 107-30-2
Molecular Formula: C_2H_5ClO, $ClCH_2$-O-CH_3
Molecular Weight: 80.513
Melting Point (°C):
–103.5 (Verschueren 1983; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
59.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.0703 (Dean 1985)
1.0605 (Budavari 1989)
Molar Volume (cm^3/mol):
75.2 (20°C, calculated-density)
81.8 (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):
decomposes (Verschueren 1983)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
24900 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.259 – 1240/(–43.15 + T/K); temp range 290–332 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

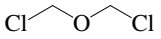
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: photooxidation $t_{½}$ = 22.7–227 h, based on estimated rate constant for the reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: k = 21 h^{-1} at pH 7 and 25°C with a calculated $t_{½}$ = 2.0 min (Van Duuren et al. 1972; quoted, Ellington 1989);
$t_{½}$ = 0.0108–0.033 h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991);
hydrolyzed very fast in aqueous solutions with $t_{½}$ < 1.0 s (Verschueren 1983).
Biodegradation: aqueous aerobic $t_{½}$ = 168–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (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: $t_{½}$ = 22.7–227 h, based on estimated rate constant for the reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: $t_{½}$ = 0.0108–0.033 h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).
Ground water: $t_{½}$ = 0.0108–0.033 h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 0.0108–0.033 h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).
Biota:

10.1.2.3 Bis(chloromethyl)ether



Common Name: Bis(chloromethyl)ether
Synonym: BCME, Bis-CME, chloro(chloromethoxy)methane, dichloromethylether, (dichloro-dimethyl)ether, sym-dichloromethyl ether, oxybis(chloromethane)
Chemical Name: chloromethyl ether, sym-dichloromethyl ether
CAS Registry No: 542-88-1
Molecular Formula: $C_2H_4Cl_2O$, $ClCH_2$-O-CH_2Cl
Molecular Weight: 114.958
Melting Point (°C):
–41.5 (Weast 1977; Weast 1982–83; Verschueren 1983; Howard 1989; Lide 2003)
Boiling Point (°C):
106 (Lide 2003)
Density (g/cm^3 at 20°C):
1.328 (15°C, Weast 1982–83)
1.315 (Verschueren 1983)
Molar Volume (cm^3/mol):
102.7 (calculated-Le Bas method at normal boiling point)
87.4 (calculated-density, Stephenson & Malanowski 1987)
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):
22000 (calculated as per Moriguchi 1975 using Quayle 1953 data, Callahan et al. 1979)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3999 (22°C, Dreisbach 1952)
$\log (P/mmHg) = -3.4945 - 2.2305 \times 10^3/(T/K) + 6.774 \cdot \log (T/K) - 1.7332 \times 10^{-2} \cdot (T/K) + 9.5511 \times 10^{-6} \cdot (T/K)^2$; temp range 232–579 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
21.27 (calculated-P/C, Mabey et al. 1982)
21.27 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
213.18 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.38 (calculated, Radding et al. 1977)
2.40 (calculated, Mabey et al. 1982)

Bioconcentration Factor, log BCF:
1.041 (bluegill sunfish, Veith et al. 1980)

Sorption Partition Coefficient, log K_{OC}:
1.20 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

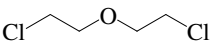
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: $k << 360$ M^{-1} h^{-1} for singlet oxygen and $k = 3.0$ M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982)
photooxidation $t_{½} = 0.196$–1.96 h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: hydrolyzed very fast in aqueous solution with half-life in the order of 10 s when extrapolated to pure water (Hammond & Alexander 1972; quoted, Verschueren 1983);
rate constant $k = 0.018\ s^{-1}$ with $t_{½} = 38$ s (Tou et al. 1974; quoted, Callahan et al. 1979; Howard et al. 1991);
hydrolysis $t_{½} = 10–38$ s and will rapidly disappear from any aquatic system (Fishbein 1979; quoted, Howard 1989);
$k = 65\ h^{-1}$ at pH 7.0 at 20°C (quoted, Mabey et al. 1982).
Biodegradation: aqueous aerobic $t_{½} = 168–672$ h, based on scientific judgement; aqueous anaerobic $t_{½} = 672–2688$ h, based on 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: $t_{½} = 0.196–1.96$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: $t_{½} = 0.0106–0.106$ h, based on estimated hydrolysis half-life in water (Howard et al. 1991).
Ground water: $t_{½} = 0.0106–0.106$ h, based on estimated hydrolysis in water (Howard et al. 1991).
Sediment:
Soil: $t_{½} < 10$ d, via volatilization subject to plant uptake from the soil (Ryan et al. 1988);
$t_{½} = 0.0106–0.106$ h, based on estimated hydrolysis half-life in water (Howard et al. 1991).
Biota:

10.1.2.4 Bis(2-chloroethyl)ether



Common Name: Bis(2-chloroethyl)ether
Synonym: 2-chloroethyl ether, 1,1′-oxybis(2-chloroethane), bis(β-chloroethyl)ether, Chlorex, 1-chloro-2-(β-chloroethoxy)-ethane, β,β′-dichloroethyl ether, 2,2′-dichloroethyl ether, di(2-chloroethyl)ether, di(chloroethyl)ether, dichlorodiethyl ether, sym-dichlorodiethyl ether
Chemical Name: 2-chloroethyl ether, bis(β-chloroethyl)ether, 1-chloro-2-(β-chloroethoxy)-ethane
CAS Registry No: 111-44-4
Molecular Formula: $C_4H_8Cl_2O$, $ClCH_2CH_2$-O-CH_2CH_2Cl
Molecular Weight: 143.012
Melting Point (°C):
–51.9 (Lide 2003)
Boiling Point (°C):
178.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.2200 (Verschueren 1983)
1.2192 (Dean 1985; Riddick et al. 1986)
Molar Volume (cm^3/mol):
117.3 (20°C, calculated-density)
147.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
8.66 (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):
10200 (20°C, Du Pont 1966; Verschueren 1983)
17195 (shake flask-LSC, Veith et al. 1980)
10200 (20°C, Riddick et al. 1986)
10400*, 10300 (20°C, 31°C, shake flask-GC/TC, measured range 0–91.7°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
156.2 (Antoine eq. regression, temp range 23.5–178.5°C, Stull 1947)
94.64, 186 (20, 25°C, Verschueren 1977,1983)
207 (selected, Riddick et al. 1986)
log (P/kPa) = 7.2289 – 2359.6/(T/K), temp range not specified (Antoine eq., Riddick et al. 1986)
143.6 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.7637 – 1948.62/(–41.974 + T/K): temp range 297–452 K (Antoine eq., Stephenson & Malanowski 1987)
857.1 (calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
28.97 (calculated-P/C, Lyman et al. 1982; Howard 1989)
1.320 (20°C, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:
1.58 (calculated, Leo et al. 1971)
1.12 (shake flask-LSC, Veith et al. 1980)
1.29 (shake flask, Hansch & Leo 1985)
1.29 (recommended, Sangster 1993)
1.29 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.041 (bluegill sunfish, Barrows et al. 1980)
1.040 (bluegill sunfish, LSC-^{14}C, Veith et al. 1980; Veith & Kosian 1983)
0.964 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
1.15 (calculated, Sabljic 1987)

Sorption Partition Coefficient, log K_{OC}:

1.38 (soil, calculated-S, Lyman et al. 1982)
1.14 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

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

Volatilization: calculated $t_{½}$ = 5.78 d (as per Mackay & Wolkoff 1973 by Durkin et al. 1975);
$t_{½}$ = 3.5, 4.4 and 180.5 d for the streams, rivers and lakes, respectively, were estimated using Henry's law constant (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{½}$ = 4.0 h, based on an estimated half-life for ethyl ether in the smog chamber (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);
$k << 360\ M^{-1} \cdot h^{-1}$ for the reaction with singlet oxygen and $k = 24.0\ M^{-1}\ h^{-1}$ for the reaction with peroxy radical (Mabey et al. 1982);
photooxidation $t_{½}$ = 9.65–96.5 h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $t_{½}$ = 40.0 d was estimated at pH 7 from ethyl chloride data in water at an unspecified temperature (Brown et al. 1975; quoted, Howard 1989);
$t_{½}$ = 0.5–2.0 yr, based on data from chlorinated ethanes and propanes (Dilling et al. 1975; quoted, Callahan et al. 1979);
first-order hydrolysis $t_{½}$ = 22 yr, based on neutral hydrolysis rate constant at 20°C which was extrapolated from data for hydrolysis of dioxane at 100°C (Mabey et al. 1982; quoted, Howard et al. 1991);
$k = 2.6 \times 10^{-5}\ h^{-1}$ at pH 7 and 25°C with a calculated $t_{½}$ = 3.0 yr (Ellington et al. 1987; quoted, Ellington 1989).

Biodegradation: aqueous aerobic $t_{½}$ = 672–4320 h, based on river die-away test data (Ludzack & Ettinger 1963 and Doljido 1979; 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: $k = 3 \times 10^{-9}$ mL cell^{-1} h^{-1} for the bacterial transformation in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: atmospheric $t_{½}$ = 13.44 h was estimated for the reaction with OH radical (GEMS 1986; quoted, Howard 1989);
photooxidation $t_{½}$ = 9.65–96.5 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 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: $t_{½} > 4.0$ d but less than 7.0 d in fish tissues (Barrows et al. 1980).

TABLE 10.1.2.4.1
Reported aqueous solubilities of bis(2-chloroethyl) ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	S/g·m^{-3}
0	11400
9.6	10900
20	10400
31	10300
40	10500
50.1	11100
60.7	11100
70.6	12800
80.9	13600
91.7	15100

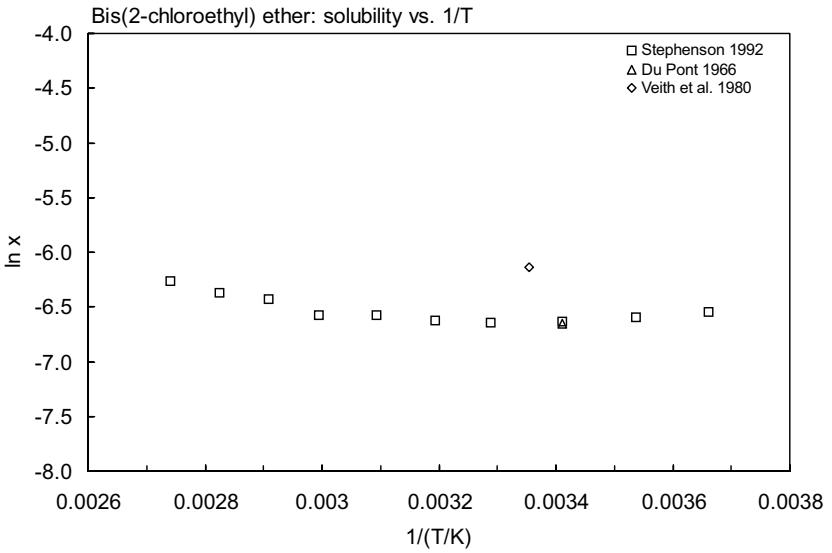
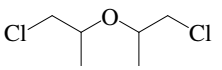


FIGURE 10.1.2.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for bis(2-chloroethyl)ether.

10.1.2.5 Bis(2-chloroisopropyl)ether



Common Name: Bis(2-chloroisopropyl)ether
Synonym: bis(2-chloro-1-methylethyl)ether, dichlorodiisopropyl ether, dichloroisopropyl ether, 2,2′-dichloroisopropyl ether, 2,2′-oxybis(1-chloropropane)
Chemical Name: bis(2-chloroisopropyl)ether, dichlorodiisopropyl ether, dichloroisopropyl ether
CAS Registry No: 108-60-1
Molecular Formula: $C_6H_{12}Cl_2O$, $ClCH_2CH(CH_3)$-O-$CH(CH_3)CH_2Cl$
Molecular Weight: 171.064
Melting Point (°C):
–97 (Weast 1977; Verschueren 1983)
Boiling Point (°C):
187 (Lide 2003)
Density (g/cm^3 at 20°C):
1.1100 (Verschueren 1983)
1.1122 (Dean 1985)
Molar Volume (cm^3/mol):
154.1 (20°C, calculated-density)
193.4 (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. Additional data at other tempertures designated * are compiled at the end of this section):
1700* (room. temp., Verschueren 1977,1983)
2450*, 2370 (19.1°C, 31.0°C, shake flask-GC, measured range 9.5–91.4°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
103.95 (Antoine eq. regression, temp range 24.7–180°C, Stull 1947)
113.31 (20°C, Verschueren 1977,1983)
112.30 (28.85°C, Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.68233 - 1856.14/(-58.793 + T/K)$; temp range 302–456 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
11.14 (20°C, calculated-P/C, Mabey et al. 1982)
11.40 (calculated-P/C from Verschueren 1977/83 data)
116.5 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
2.58 (calculated, Leo et al. 1971)
2.10 (calculated, Mabey et al. 1982)
2.48 (HPLC-RT correlation, Kawamoto & Urano 1989)
2.48 (recommended, Sangster 1993)

Bioconcentration Factor, log BCF:
1.544 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
1.785 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

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

Volatilization: calculated $t_{½}$ = 1.37 d (calculated as per Mackay & Wolkoff 1973, Durkin et al. 1975; quoted, Callahan et al. 1979).

Photolysis:

Oxidation: photooxidation $t_{½}$ = 4.0 h, based on estimated half-life for ethyl ether in a smog chamber (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);

$k << 360\ M^{-1}\ h^{-1}$ for the reaction with singlet oxygen and $k = 2.0\ M^{-1}\ h^{-1}$ for the reaction with peroxy radical (Mabey et al. 1982).

Hydrolysis: $t_{½}$ = 0.5–2.0 yr, based on data from chlorinated ethanes and propanes (Dilling et al. 1975; quoted, Callahan et al. 1979);

$k = 4 \times 10^{-6}\ h^{-1}$ at pH 7.0 and 25°C (Mabey et al. 1982).

Biodegradation: aqueous aerobic $t_{½}$ = 432–4320 h, based on river die-away test data (Kleopfer & Fairless 1972; quoted, Howard et al. 1991) and aerobic soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 1728–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $k = 1 \times 10^{-10}$ mL cell^{-1} h^{-1} for bacterial transformation in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: $t_{½}$ = 4.61–46.1 h, based on photooxidation half-life in air (Howard et al. 1991).

Surface water: estimated $t_{½}$ = 3.1 d for surface waters in case of a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{½}$ = 432–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{½}$ = 864–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 432–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 10.1.2.5.1
Reported aqueous solubilities of bis(2-chloroisopropyl) ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	S/g·m^{-3}
9.5	4090
19.1	2450
31	2370
40.3	2180
51.1	1820
60.6	2090
80.7	2650
91.4	2410

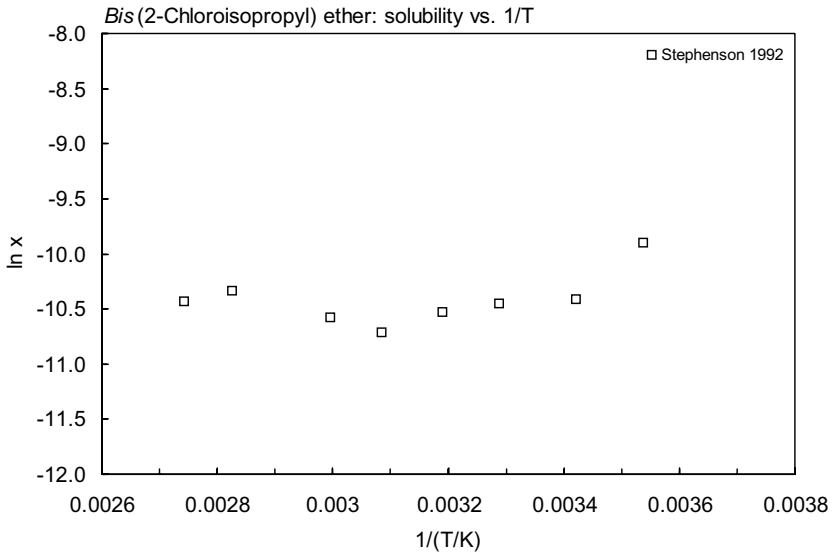
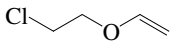


FIGURE 10.1.2.5.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for bis(2-chloroisopropyl)ether.

10.1.2.6 2-Chloroethyl vinyl ether



Common Name: 2-Chloroethyl vinyl ether
Synonym: (2-chloroethoxy)-ethene, β-chloroethyl vinyl ether, vinyl 2-chloroethyl ether
Chemical Name: β-chloroethyl vinyl ether, 2-chloroethyl vinyl ether, vinyl 2-chloroethyl ether
CAS Registry No: 110-75-8
Molecular Formula: $C_4H_7Cl_2O$, $ClCH_2CH_2$-O-$CH{=}CH_2$
Molecular Weight: 106.551
Melting Point (°C):
–70 (Lide 2003)
Boiling Point (°C):
108 (Weast 1977; Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.0475 (Weast 1982–83)
1.0480 (Dean 1985)
Molar Volume (cm^3/mol):
101.7 (20°C, calculated-density)
119.6 (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 (calculated as per Moriguchi 1975, Callahan et al.)
6000 (Dean 1985)

Vapor Pressure (Pa at 25°C or as indicated):
3566 (20°C, calculated, Dreisbach 1952)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
0.0253 (20–25°C, calculated-P/C, Mabey et al. 1982)
25.33 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
24.79 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
1.28 (calculated as per Leo et al. 1971, Callahan et al. 1979)
1.14 (calculated, Mabey et al. 1982)

Bioconcentration Factor, log BCF:
0.672 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

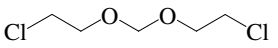
Sorption Partition Coefficient, log K_{OC}:
0.820 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: photooxidation $t_{½}$ = 30 min, based on half-life estimated for 2-methyl-2-butene from smog chamber data (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);
$k = 1 \times 10^{10}$ $M^{-1} \cdot h^{-1}$ for singlet oxygen and $k = 34$ M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982).
Hydrolysis: $k = 4.4 \times 10^{-10}$ s^{-1}, minimum rate at pH 7 and 25°C in pure water with a maximum $t_{½}$ = 0.48 yr (Jones & Wood 1964; quoted, Callahan et al. 1979);
$k \sim 4 \times 10^{-6}$ h^{-1} at pH 7.0 and 25°C with reference to that of bis(2-chloroethyl)ether (Mabey et al. 1982).

Biodegradation:
Biotransformation: $k = 1 \times 10^{-10}$ mL cell^{-1} h^{-1} for bacterial transformation to water (Mabey et al. 1982).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Soil: $t_{½} < 10$ d, via volatilization subject to plant uptake from the soil (Ryan et al. 1988).

10.1.2.7 Bis(2-chloroethoxy)methane



Common Name: Bis(2-chloroethoxy)methane
Synonym: bis(β-chloroethyl)formal, β, β-dichlorodiethyl formal, dichlorodiethyl methylal
Chemical Name: bis(2-chloroethoxy)methane
CAS Registry No: 111-91-1
Molecular Formula: $C_5H_{10}Cl_2O_2$, $ClCH_2CH_2$-O-CH_2-O-CH_2CH_2Cl
Molecular Weight: 173.037
Melting Point (°C):
Boiling Point (°C):
215 (Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
180.0 (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: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
81000 (calculated as per Moriguchi 1975, Callahan et al. 1979;)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
21.58 (Antoine eq. regression, temp range 53–215°C, Stull 1947)
< 13.3 (calculated as per Dreisbach 1952 using data of Webb et al. 1962, Callahan et al. 1979)
21.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.54778 – 2641.33/(–11.518 + T/K); temp range 326–486 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
0.0284 (20–25°C, calculated-P/C, Mabey et al. 1982)
0.0273 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
1.260 (calculated as per Leo et al. 1971, Callahan et al. 1979; Ryan et al. 1988)
1.029 (calculated, Mabey et al. 1982)

Bioconcentration Factor, log BCF:
0.568 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
0.716 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

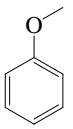
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: k << 360 M^{-1} h^{-1} for singlet oxygen and k = 52 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982).
Hydrolysis: minimum rate k = 2.53 × 10^{-6} L mol^{-1} s^{-1} for acid-catalyzed hydrolysis of the acetal linkage at 25°C (Kankaanperä 1969; quoted, Callahan et al. 1979; Mabey et al. 1982);
$t_{½}$ = 0.5–2.0 yr, based on data of Dilling et al. 1975 on chlorinated ethanes and propanes (quoted, Callahan et al. 1979);
estimated rate constant k ~ 4 × 10^{-6} h^{-1} at pH 7.0 and 25°C by analogy to bis(2-chloroethyl)ether (Mabey et al. 1982).

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

Half-Lives in the Environment:
Soil: $t_{½} > 50$ d, via volatilization subject to plant uptake from the soil (Ryan et al. 1988).

10.1.3 Aromatic ethers

10.1.3.1 Anisole (Methoxybenzene)



Common Name: Anisole
Synonym: methoxybenzene
Chemical Name: anisole, methoxybenzene, methyl phenyl ether
CAS Registry No: 100-66-3
Molecular Formula: C_7H_8O, $C_6H_5OCH_3$
Molecular Weight: 108.138
Melting Point (°C):
–37.13 (Lide 2003)
Boiling Point (°C):
153.7 (Lide 2003)
Density (g/cm^3 at 20°C):
0.99402, 0.98932 (20°C, 25°C, Dreisbach & Martin 1949)
0.9940, 0.9893 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
108.8 (20°C, calculated-density)
127.3 (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 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
1514 (shake flask-UV, McGowan et al. 1966)
1536 (shake flask-UV, Vesala 1974)
2030*, 1860 (20°C, 29.7°C, shake flask-GC/TC, measured range 0–90.7°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):
497* (calculated-Antoine eq. regression, temp range 5.4–155.5°C, Stull 1947)
log (P/mmHg) = 7.35950 – 1718.7/(230 + t/°C) (Antoine eq., temp range 73–154°C, Dreisbach & Martin 1949)
6287* (73.34°C, ebulliometry, measured range 73.34–153.75°C, Dreisbach & Shrader 1949)
26547* (109.876°C, ebulliometry, measured range 109.876–164.114°C, Collerson et al. 1965)
log (P/mmHg) = 7.05236 – 1489.756/(203.543 + t/°C); temp range 109.876–164.114°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = 22.84299 – 3033.20/(T/K) – 4.88720·log (T/K); temp range 109.876–164.114°C (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = [–0.2185 × 10440.9/(T/K)] + 8.221443; temp range 5.4–155.5°C (Antoine eq., Weast 1972–73)
472* ("recomputed" reported data, ebulliometry, measured range 383–437 K, Ambrose et al. 1976)
log (P/kPa) = 6.17595 – 1489.502/(T/K – 69.577); temp range 383–437 K (Antoine eq., ebulliometry, Ambrose et al. 1976)
log (P/mmHg) = [1 – 426.827/(T/K)] × 10^{0.942238 – 10.2065 × 10^{-4}·(T/K) + 10.6819 × 10^{-7}·(T/K)^2}; temp range 346.49–415.52 K (Cox eq., Chao et al. 1983)
log (P/kPa) = 6.23361 – 1529.735/(208.062 + t/°C); temp range 73.3–153.75°C (Antoine eq. derived from exptl data of Dreisbach & Shrader 1949, Boublik et al. 1984)
log (P/kPa) = 6.17900 – 1490.93/(203.675 + t/°C); temp range 109.9–164.1°C (Antoine eq. derived from reported exptl data of. Collerson et al. 1965, Boublik et al. 1984)

log (P/mmHg) = 7.05269 – 1489.99/(203.57 + t/°C); temp range 110–164°C (Antoine eq., Dean 1985, 1992)
472 (selected, Riddick et al. 1986)
log (P/kPa) = 6.17595 – 1489.502/(203.573 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
log (P_L/kPa) = 6.17622 – 1489.957/(–69.525 + T/K); temp range 382–437 K (Antoine eq., Stephenson & Malanowski 1987)
204, 383 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
log (P/mbar) = 7.11773 – 1451.742/[(T/K) –73.252]; temp range 382–429 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)
log (P/mmHg) = $-8.1053 - 2.5386 \times 10^3/(T/K) + 9.0289 \cdot \log(T/K) - 2.0426 \times 10^{-2} \cdot (T/K) + 1.0536 \times 10^{-5} \cdot (T/K)^2$; temp range 236–642 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
430.8 (exptl. $1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975)
430.8, 358.3 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:
2.11 (shake flask-UV, Fujita et al. 1964)
2.04 (shake flask-UV, Rogers & Cammarata 1969)
2.10 (HPLC-RT correlation, Mirrlees et al. 1976)
2.08 (Hansch & Leo 1979)
2.24 (HPLC-k′ correlation, Haky & Young 1984)
2.16 (HPLC-RT correlation, Ge et al. 1987)
2.15 (HPLC-RT correlation, Minick et al. 1988)
2.01 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
2.11 (recommended, Sangster 1989, 1993)
2.17 (dual-mode centrifugal partition chromatography, Gluck 1990)
1.67, 1.79 (shake flask-UV/VIS spec.: 25, 60°C, Kramer & Henze 1990)
2.11 (recommended, Hansch et al. 1995)
2.41, 2.31, 2.58, 2.55 (HPLC-k′ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovsakya et al. 1995)

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

Bioconcentration Factor, log BCF:
1.34 (Isnard & Lambert 1988)

Sorption Partition Coefficient, log K_{OC}:
6.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis: rate constant $k = 1.054 \times 10^{-2}$ 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:
$k_{OH} = (1.57 \pm 0.24) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 299 K, measured range 299–435 K (overall rate constant, flash photolysis-resonance fluorescence technique, Perry et al. 1977)
$k_{OH} = 1.57 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (Atkinson 1985; quoted, Sabljic & Güsten 1990)
$k_{NO3} = 9.0 \times 10^{-17}$ cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K (re-evaluated value, Atkinson et al. 1987)
$k_{OH} = 1.35 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} in air, extrapolated from lit. data to 25°C (Dilling et al. 1988)
$k_{NO3} = 2.08 \times 10^{-16}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)
$k_{OH} = (14.1 - 19.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. to 299.9 K (Atkinson 1989)
Hydrolysis:
Biodegradation:

Biotransformation: degradation $k = 2.86 \times 10^{-17}$ mol cell^{-1} h^{-1} in pure culture system (Banerjee et al. 1984).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{½} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.3.1.1
Reported aqueous solubilities of anisole at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	**S/g·m^{-3}**
0	
10.2	2370
20	2030
29.7	1860
39.9	1840
50.2	1990
60.2	2550
70.2	2530
81.2	2940
90.7	3520

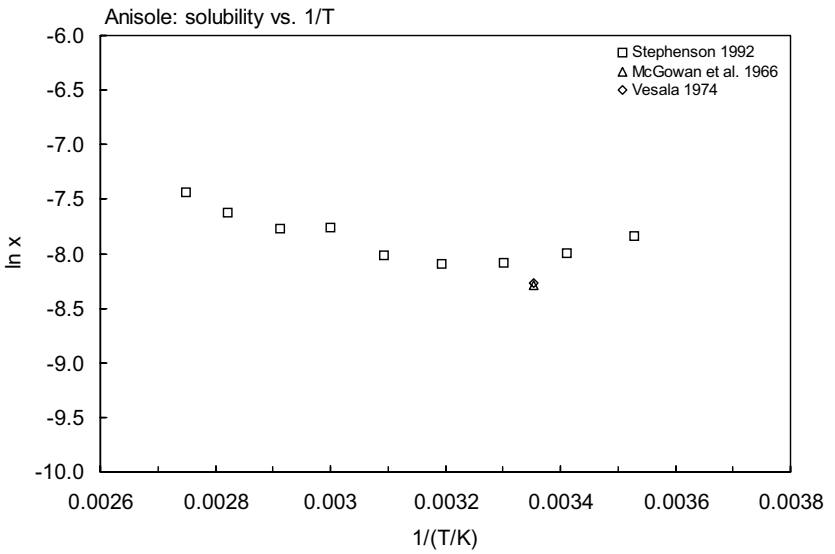


FIGURE 10.1.3.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for anisole.

TABLE 10.1.3.1.2
Reported vapor pressures of anisole 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		**Dreisbach & Shrader 1949**		**Collerson et al. 1965**		**Ambrose et al. 1976**	
summary of literature data		**ebulliometry**		**ebulliometry**		**comparative ebulliometry**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
5.4	133.3	73.34	6287	109.876	26547	109.88	26547
30	666.6	81.31	8851	116.255	33024	116.261	33024
42.2	1333	84.55	10114	122.045	39966	122.053	39966
55.8	2666	99.89	16500	126.854	46587	126.864	46587
70.7	5333	123.77	42066	131.266	55425	131.279	53424
80.1	7999	139.37	67661	136.078	59950	135.092	59950
93	13332	153.75	101325	138.64	66614	138.655	66614
112.3	26664			141.919	73266	141.936	73266
133.8	53329			145.003	79992	145.021	79992
155.5	101325	Antoine eq. given by		147.89	86731	147.91	86732
		Dreisbach & Martin 1949		150.429	93021	150.45	93021
mp/°C	–37.3	Eq. 2	P/mmHg	153.143	100135	153.164	100137
		A	7.3595	155.554	106819	155.576	106820
		B	1718.7	157.81	113382	157.834	113381
		C	230	160.009	120086	160.033	120084
				162.087	126698	162.113	126697
		bp/°C	153.75	164.114	133429	164.141	133427
		mp/°C	–37.38			25	472
				bp/°C	153.598		
						Antoine eq.	
				Antoine eq.		eq. 2	P/kPa
				eq. 2	P/mmHg	A	6.17595
				A	705236	B	1489.502
				B	1489.756	C	–69.577
				C	203.543		
				Kirchhoff eq.		Coefficients of Chebyshev eq. are	
				eq. 4	P/mmHg	also given in text.	
				A	22.842 99		
				B	3033.2		
				C	4.8872		
				ΔH_v/(kJ mol^{-1}) = 39.04			

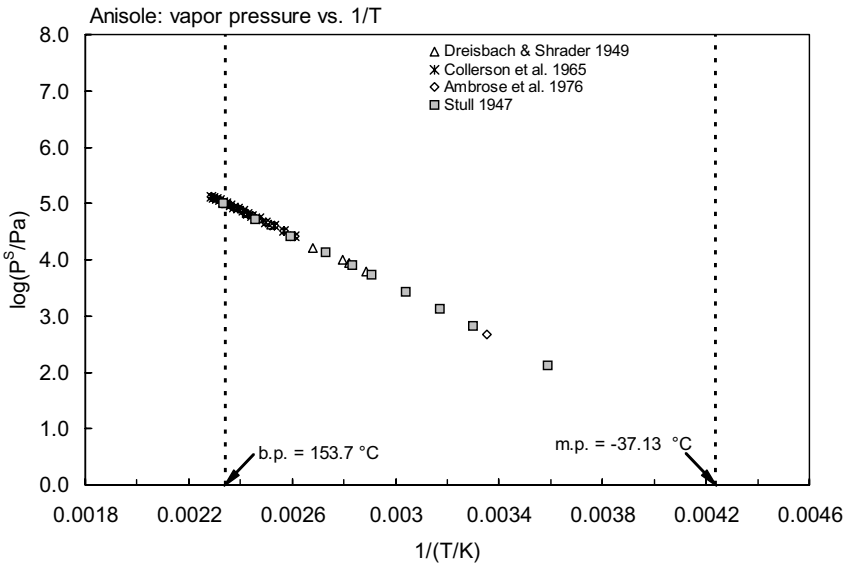
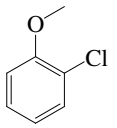


FIGURE 10.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for anisole.

10.1.3.2 2-Chloroanisole



Common Name: 2-Chloroanisole
Synonym: 1-chloro-2-methoxybenzene
Chemical Name: 2-chloroanisole
CAS Registry No: 766-51-8
Molecular Formula:C_7H_7ClO, $C_6H_4Cl(OCH_3)$
Molecular Weight: 142.583
Melting Point (°C): liquid
–26.8 (Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
198.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.1911 (Lide 2003)
Molar Volume (cm^3/mol):
119.7 (20°C, calculated-density)
148.2 (Le Bas method-calculated 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: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
490 (shake flask-HPLC/UV, Lun et al. 1995)
766 (liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
6287 (115.13°C, ebulliometry, measured range 115.13–186.19°C, Dreisbach & Shrader 1949)
log (P/mmHg) = 7.54073 – 2012.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
log (P/kPa) = 6.25236 – 1660.008/(189.207 + t/°C), temp range 115.13–186.19°C (Antoine eq. derived from exptl data of Dreisbach & Shrader 1949, Boublik et al. 1984)
0.0594 (P_L, extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.66563 – 2012.4/(–43.15 + T/K), temp range 388–460 K, (Antoine eq., Stephenson & Malanowski 1987)
0.0302 (liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
9.50 (calculated-P_L/C_L, Pfeifer et al. 2001)

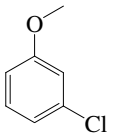
Octanol/Water Partition Coefficient, log K_{OW}:
2.68 (shake flask-UV, Nakagawa et al. 1992)
2.50 (shake flask-HPLC/UV both phases, Lun et al. 1995)
2.72 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
3.13 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

10.1.3.3 3-Chloroanisole



Common Name: 3-Chloroanisole
Synonym:
Chemical Name:
CAS Registry No: 2845-89-8
Molecular Formula:C_7H_7ClO, $C_6H_4Cl(OCH_3)$
Molecular Weight: 142.583
Melting Point (°C): liquid
Boiling Point (°C):
193.5 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
148.2 (Le Bas method-calculated 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: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
235 (shake flask-HPLC/UV, Lun et al. 1995)
231 (liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C):
0.0282 (liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
21.4 (calculated-P_L/C_L, Pfeifer et al. 2001)

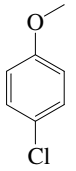
Octanol/Water Partition Coefficient, log K_{OW}:
2.60 (shake flask-HPLC/UV both phases, Lun et al. 1995)
3.09 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
3.15 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

10.1.3.4 4-Chloroanisole



Common Name: 4-Chloroanisole
Synonym: 1-chloro-4-methoxy-benzene
Chemical Name: 4-chloroanisole
CAS Registry No: 623-12-1
Molecular Formula: C_7H_7ClO, $C_6H_4Cl(OCH_3)$
Molecular Weight: 142.583
Melting Point (°C):
< –18 (Lide 2003)
Boiling Point (°C):
197.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.201 (Lide 2003)
Molar Volume (cm^3/mol):
118.7 (20°C, calculated-density)
148.2 (Le Bas method-calculated 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):
237 (shake flask-HPLC/UV, Lun et al. 1995)
312 (liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C):
0.0324 (liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
18.2 (calculated-P_L/C_L, Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
2.78 (23°C, shake flask-LSC, Banerjee et al. 1980)
2.78 (recommended, Sangster 1993)
2.70 (shake flask-HPLC/UV both phases, Lun et al. 1995)
3.00 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
3.13 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

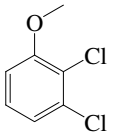
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Biodegradation: degradation rate constants k = 2.29×10^{-18} mol cell^{-1} h^{-1} from pure culture studies (Banerjee et al. 1984).

Half-Lives in the Environment:

10.1.3.5 2,3-Dichloroanisole



Common Name: 2,3-Dichloroanisole
Synonym:
Chemical Name:
CAS Registry No: 1984-59-4
Molecular Formula: $C_7H_6Cl_2O$, $C_6H_3Cl_2(OCH_3)$
Molecular Weight: 177.028
Melting Point (°C):
32 (Lun et al. 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
169.1 (Le Bas method-calculated 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: 0.854 (mp at 32°C)

Water Solubility (g/m^3 or mg/L at 25°C):
86.9 (shake flask-GC/ECD, Lun et al. 1995)
140.6 (supercooled liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C):
0.0468 (supercooled liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
44.1 (calculated-P_L/C_L, Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
3.24 (shake flask-HPLC/UV both phases, Lun et al. 1995)
3.30 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
3.05 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

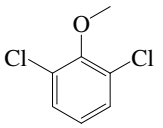
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.3.6 2,6-Dichloroanisole



Common Name: 2,6-Dichloroanisole
Synonym:
Chemical Name:
CAS Registry No: 1984-65-2
Molecular Formula: $C_7H_6Cl_2O$, $C_6H_3Cl_2(OCH_3)$
Molecular Weight: 177.028
Melting Point (°C):
10 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
169.1 (Le Bas method-calculated 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):
13.12 (shake flask-GC/ECD, Lun et al. 1995)
21.8 (liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C):
0.0110 (liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
113.7 (calculated-P_L/C_L, Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
2.96 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
3.14 (shake flask-HPLC/UV both phases, Lun et al. 1995)
3.10 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
2.53 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

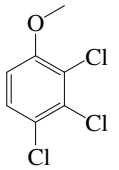
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.3.7 2,3,4-Trichloroanisole



Common Name: 2,3,4-Trichloroanisole
Synonym:
Chemical Name:
CAS Registry No: 54135-80-7
Molecular Formula: $C_7H_5Cl_3O$, $C_6H_2Cl_3(OCH_3)$
Molecular Weight: 211.473
Melting Point (°C):
70 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
190.0 (Le Bas method-calculated 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: 0.362 (mp at 70°C)

Water Solubility (g/m^3 or mg/L at 25°C):
10.8 (shake flask-GC/ECD, Lun et al. 1995)
22.1 (supercooled liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C):
0.263 (supercooled liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
74.7 (calculated-P_L/C_L, Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
3.74 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
4.03 (shake flask-GC/ECD, both phases, Lun et al. 1995)
3.92 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
3.44 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

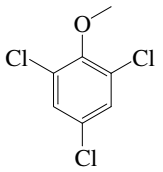
Bioconcentration Factor, log BCF or log K_B:
3.09 (guppy, concn ratio of C_{fish}/C_{water}, Opperhuizen & Voors 1987)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$, or Lifetimes, τ:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 1450 mL g^{-1} d^{-1}; k_2 = 1.9 d^{-1} (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

10.1.3.8 2,4,6-Trichloroanisole



Common Name: 2,4,6-Trichloroanisole
Synonym:
Chemical Name:
CAS Registry No: 87-40-1
Molecular Formula: $C_7H_5Cl_3O$, $C_6H_2Cl_3(OCH_3)$
Molecular Weight: 211.473
Melting Point (°C): 61.5 (Lide 2003)
Boiling Point (°C): 241 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
190.0 (Le Bas method-calculated 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: 0.438 (mp at 61.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
13.2 (shake flask-GC/ECD, Lun et al. 1995)
14.6 (supercooled liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C):
2.065 (GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0724 (supercooled liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
218.7 (calculated-P_L/C_L, Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
5.20 (HPLC-relative retention time correlation, Neilson et al. 1984)
4.11 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
3.96 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
4.02 (shake flask-GC/ECD, both phases, Lun et al. 1995)
4.05 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
3.10 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

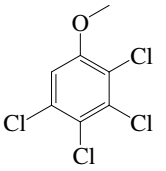
Bioconcentration Factor, log BCF or log K_B:
3.90 (zebra fish, Neilson et al. 1984)
2.86 (guppy, concn ratio of C_{fish}/C_{water}, Opperhuizen & Voors 1987)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 = 1600\ mL\ g^{-1}\ d^{-1}$; $k_2 = 2.5\ d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:
Biota: biological $t_{½} < 1$ d for all trichloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.9 2,3,4,5-Tetrachloroanisole



Common Name: 2,3,4,5-Tetrachloroanisole
Synonym:
Chemical Name:
CAS Registry No: 938-86-3
Molecular Formula: $C_7H_4Cl_4O$, $C_6HCl_4(OCH_3)$
Molecular Weight: 245.918
Melting Point (°C):
88 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
210.9 (Le Bas method-calculated 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: 0.241 (mp at 88°C)

Water Solubility (g/m^3 or mg/L at 25°C):
1.35 (shake flask-GC/ECD, Lun et al. 1995)
2.76 (supercooled liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C):
1.202 (supercooled liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
153.0 (calculated-P_L/C_L, Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
4.51 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
4.50 (shake flask-GC/ECD, both phases, Lun et al. 1995)
4.57 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
3.78 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

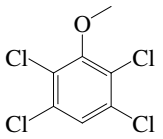
Bioconcentration Factor, log BCF or log K_B:
3.67 (guppy, concn ratio of C_{fish}/C_{water}, Opperhuizen & Voors 1987)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$, or Lifetimes, τ:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 = 940$ mL g^{-1} d^{-1}; $k_2 = 0.42$ d^{-1} (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:
Biota: biological $t_{½}$ ~ 1–4 d for all tetrachloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.10 2,3,5,6-Tetrachloroanisole



Common Name: 2,3,5,6-Tetrachloroanisole
Synonym:
Chemical Name:
CAS Registry No: 6936-40-9
Molecular Formula: $C_7H_4Cl_4O$, $C_6HCl_4(OCH_3)$
Molecular Weight: 245.918
Melting Point (°C):
84 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
210.9 (Le Bas method-calculated 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: 0.264 (mp at 84°C)

Water Solubility (g/m^3 or mg/L at 25°C):
1.82 (shake flask-GC/ECD, Lun et al. 1995)
3.64 (supercooled liquid S_L, RP-HPLC-k′ correlation, using chlorobenzene as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at 25°C):
0.427 (supercooled liquid P_L, GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
318.4 (calculated-P_L/C_L, Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
4.68 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
4.40 (shake flask-GC/ECD, both phases, Lun et al. 1995)
4.52 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
3.41 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)

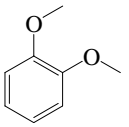
Bioconcentration Factor, log BCF or log K_B:
3.69 (guppy, concn ratio of C_{fish}/C_{water}, Opperhuizen & Voors 1987)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$, or Lifetimes, τ:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 1480 mL g^{-1} d^{-1}; k_2 = 0.44 d^{-1} (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:
Biota: biological $t_{½}$ ~ 1–4 d for all tetrachloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.11 Veratrole (1,2-Dimethoxybenzene)



Common Name: Veratrole
Synonym: 1,2-dimethoxybenzene
Chemical Name: 1,2-dimethoxybenzene
CAS Registry No: 91-16-7
Molecular Formula: $C_8H_{10}O_2$, $C_6H_4(OCH_3)_2$
Molecular Weight: 138.164
Melting Point (°C):
22 (Stephenson & Malanowski 1987)
22.5 (Lide 2003)
Boiling Point (°C):
206.7 (Stephenson & Malanowksi 1987)
206 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
127.1 (calculated-density)
158.6 (Le Bas method-calculated 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):
7160*, 7060 (19.9, 31°C, shake flask-GC, measured range 19.9–91.8°C, Stephenson 1992)
6690 (shake flask-HPLC/UV, Lun et al. 1995)

Vapor Pressure (Pa at 25°C):
log (P_L/kPa) = 8.705 – 3492/(T/K), temp range not specified (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
1.79 (Log P Database, Hansch & Leo 1987, quoted, Sangster 1993)
1.79 (HPLC-RT correlation, average value, Ritter et al. 1994)
1.60 (recommended, Hansch et al. 1995)
2.18 (shake flask-HPLC/UV both phases, Lun 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 10.1.3.11.1
Reported aqueous solubilities of veratrole at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	S/g·m^{-3}
19.9	7160
31	7060
41.1	7230
50.6	7580
60.2	7940
70.6	8770
80.7	9700
91.8	10730

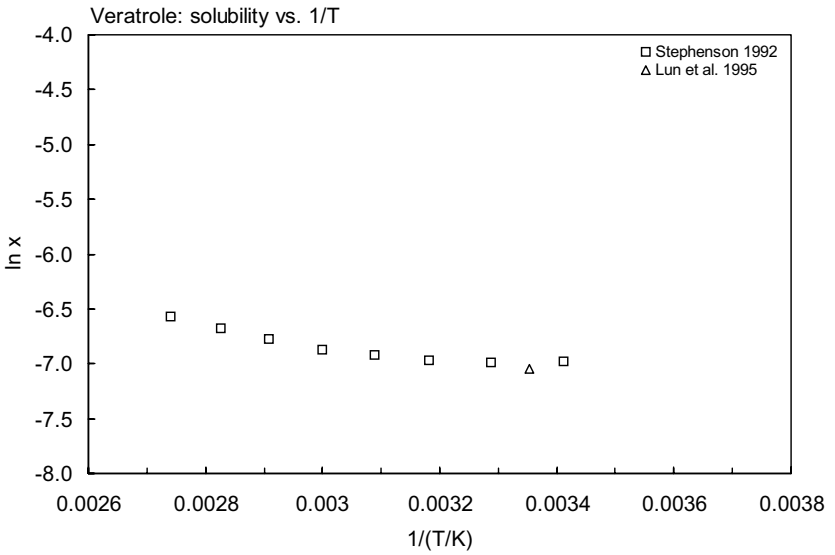
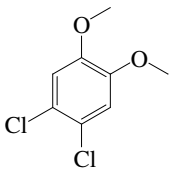


FIGURE 10.1.3.11.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for veratrole.

10.1.3.12 4,5-Dichloroveratrole



Common Name: 4,5-dichloroveratrole
Synonym:
Chemical Name:
CAS Registry No: 2772-46-5
Molecular Formula: $C_8H_8Cl_2O_2$, $C_6H_2Cl_2(OCH_3)_2$
Molecular Weight: 207.054
Melting Point (°C):
83 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
200.4 (Le-Bas method-calculated 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: 0.27 (mp at 83°C)

Water Solubility (g/m^3 or mg/L at 25°C):
71.9 (shake flask-HPLC/UV, Lun et al. 1995)
72.6 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
3.11 (shake flask-GC/ECD, both phases, Lun et al. 1995)

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

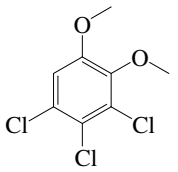
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.3.13 3,4,5-Trichloroveratrole



Common Name: 3,4,5-trichloroveratrole
Synonym:
Chemical Name:
CAS Registry No: 16766-29-3
Molecular Formula: $C_8H_7Cl_3O_2$, $C_6HCl_3(OCH_3)_2$
Molecular Weight: 241.499
Melting Point (°C):
66 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
221.3 (Le Bas method-calculated 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: 0.396 (mp at 66°C)

Water Solubility (g/m^3 or mg/L at 25°C):
2.50 (shake flask-GC, Neilson et al. 1984)
10.3 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
4.60, 5.25 (HPLC-RT correlation, calculated-solubility, Neilson et al. 1984)
4.01 (shake flask-GC/ECD, both phases, Lun et al. 1995)

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

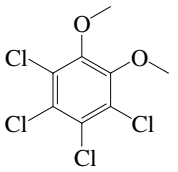
Bioconcentration Factor, log BCF or log K_B:
3.50, 3.30 (zebra fish, calculated, Neilson et al. 1984)

Sorption Partition Coefficient, log K_{OC}:
3.20 (sediment, K_P = 1.6 ml·(kg of organic C)$^{-1}$, batch sorption equilibrium, Remberger et al. 1986)

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

Half-Lives in the Environment:

10.1.3.14 Tetrachloroveratrole



Common Name: Tetrachloroveratrole
Synonym: 1,2,3,4-tetrachloro-5,6-dimethoxybenzene
Chemical Name: tetrachloroveratrole
CAS Registry No: 944-61-6
Molecular Formula: $C_8H_6Cl_4O_2$, $C_6Cl_4(OCH_3)_2$
Molecular Weight: 275.944
Melting Point (°C):
90 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
242.2 (Le Bas method-calculated 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: 0.23 (mp at 90°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.70 (shake flask-GC, Neilson et al. 1984)
1.59 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.80, 5.90 (HPLC-RT correlation, calculated-solubility, Neilson et al. 1984)
4.70 (Sarrikoski et al. 1986)
5.90 (Part et al. 1992, quoted, Sangster 1993)
4.86 (shake flask-GC/ECD both phases, Lun et al. 1995)

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

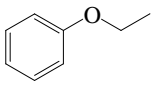
Bioconcentration Factor, log BCF or log K_B:
4.40, 4.50 (zebra fish, calculated, Neilson et al. 1984)

Sorption Partition Coefficient, log K_{OC}:
3.45 (sediment, K_P = 2.8 ml·(kg of organic C)$^{-1}$, batch sorption equilibrium, Remberger et al. 1986)

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

Half-Lives in the Environment:

10.1.3.15 Phenetole



Common Name: Phenetole
Synonym: ethoxybenzene, ethyl phenyl ether
Chemical Name: ethoxybenzene, ethyl phenyl ether
CAS Registry No: 103-73-1
Molecular Formula: $C_8H_{10}O$, C_6H_5-O-C_2H_5
Molecular Weight: 122.164
Melting Point (°C):
–29.52 (Riddick et al. 1986)
–33.00 (Stephenson & Malanowski 1987)
–29.43 (Lide 2003)
Boiling Point (°C):
169.84 (Riddick et al. 1986)
172.00 (Stephenson & Malanowski 1987)
169.81 (Lide 2003)
Density (g/cm^3 at 20°C):
0.9651, 0.9605 (20°C, 25°C, Dreisbach & Martin 1949; Riddick et al. 1986)
Molar Volume (cm^3/mol):
126.6 (20°C, calculated-density)
150.3 (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):
1160 (residual volume, Booth & Everson 1948)
550 (shake flask-AS, McGowan et al. 1966)
569 (shake flask-UV, Vesala 1974)
1114 (calculated-K_{OW}, Valvani et al. 1981)
1200 (selected, Riddick et al. 1986)

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* (18°C, compiled and evaluated data, temp range 18–172°C, Stull 1947)
log (P/mmHg) = 7.40281 – 1808.8/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
7605* (91.89°C, ebulliometry, measured range 91.89–170°C, Dreisbach & Shrader 1949)
20441* (117.43°C, ebulliometry, measured range 117.43–180.608°C, Collerson et al. 1965)
log (P/mmHg) = 7.01980 – 1507.267/(194.357 + t/°C); temp range 117.43–180.608°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = 24.97404 – 3295.20/(T/K) – 5.53743·log (T/K); temp range 117.43–180.608°C (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)
204* (comparative ebulliometry-extrapolated, measured range 117.438–180.642°C, Ambrose et al. 1976)
log (P/kPa) = 6.14658 – 1509.276/{(T/K) – 78.502}; temp range 391–454 K (Antoine eq., Ambrose et al. 1976)
log (P/kPa) = 6.17151 – 1529.38/(197.132 + t/°C); temp range 91.89–170°C (Antoine eq. derived from exptl data of Dreisbach & Martin 1949, Boublik et al. 1984)
log (P/kPa) = 6.14656 – 1508.583/(194.512 + t/°C); temp range 117.4–180.68°C (Antoine eq. derived reported exptl data of Collerson et al. 1965, Boublik et al. 1984)
204 (selected, Riddick et al. 1986)
log (P/kPa) = 6.14658 – 1509.276/(194.648 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P_L/kPa) = 6.14524 – 1508.326/(–78.613 + T/K); temp range 390–454 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = $-8.3543 - 2.7728 \times 10^3/(T/K) + 9.4482 \cdot \log (T/K) - 2.1842 \times 10^{-2} \cdot (T/K) + 1.1038 \times 10^{-5} \cdot (T/K)^2$; temp range 244–647 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

44.5 (calculated-P/C from selected data)

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

2.51 (shake flask, Hansch & Leo 1979; 1987)
2.68 (HPLC-k′ correlation, Haky & Young 1984)
2.51 (recommended, Sangster 1993)
2.51 (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:

TABLE 10.1.3.15.1
Reported vapor pressures of phenetole 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		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1976	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
18.1	133.3	91.89	7605	117.432	20441	117.438	20441
43.7	666.6	95.6	8850	124.908	26526	124.918	26526
56.4	1333	98.84	10114	131.478	33024	131.49	33024
70.3	2666	111.56	16500	137.43	39978	137.445	39978
86.6	5333	139.17	42066	142.338	46566	142.355	46566
95.4	7999	155.16	67661	146.908	53454	146.927	53453
108.4	13332	170	101325	150.795	59940	150.816	59940
127.9	26664			154.432	66655	154.455	66570
149.8	53329			157.829	73278	157.853	73277
172	101325	Antoine eq. given by		160.982	79972	161.008	79972
		Dreisbach & Martin 1949		163.972	86762	163.999	86762
mp/°C	–30.2	eq. 2	P/mmHg	166.622	93152	166.65	93152
		A	7.40281	169.315	100033	169.344	100033
		B	1808.8	171.821	106789	171.852	106788
		C	230	174.19	113487	174.221	113486
				176.407	120058	176.439	120057
		bp/°C	170	178.511	126572	178.544	126571
		mp/°C	–29.52	180.608	133334	180.642	133334
						25	204

(*Continued*)

TABLE 10.1.3.15.1 (*Continued*)

Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1976	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				bp/°C	169.806		
				Antoine eq.		Antoine eq.	
				eq. 2	P/mmHg	eq. 2	P/kPa
				A	7.0198	A	6.14658
				B	1507.267	B	1509.276
				C	194.357	C	–78.502
				Kirchhoff eq.			
				eq. 4	P/mmHg	Coefficients of Chebyshev eq.	
				A	24.97404	also given in text.	
				B	3295.2		
				C	5.53743		
				ΔH_V/(kJ mol^{-1}) = 40.71			

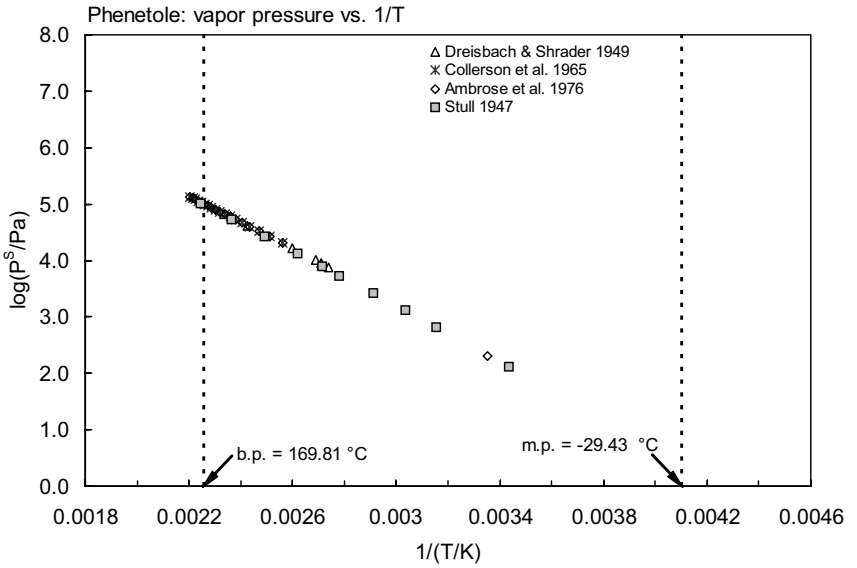
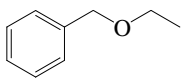


FIGURE 10.1.3.15.1 Logarithm of vapor pressure versus reciprocal temperature for phenetole.

10.1.3.16 Benzyl ethyl ether



Common Name: Benzyl ethyl ether
Synonym: (ethoxymethyl)benzene, α-ethoxytoluene
Chemical Name: benzyl ethyl ether, (ethoxymethyl)benzene, α-ethoxytoluene
CAS Registry No: 539-30-0
Molecular Formula: $C_9H_{12}O$, $C_6H_5CH_2$-O-C_2H_5
Molecular Weight: 136.190
Melting Point (°C):
Boiling Point (°C):
185.6 (Lide 2003)
Density (g/cm^3 at 20°C):
0.9490 (Weast 1982–83)
0.9478 (Dean 1985)
Molar Volume (cm^3/mol):
143.5 (20°C, calculated-density)
172.5 (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):

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):
135* (calculated-Antoine eq. regression, Stull 1947)
100 (selected, Riddick et al. 1986)
log (P/kPa) = 6.6496 – 1927.21/(230 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
135 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.92406 – 2133.29/(–24.38 + T/K); temp range 299–460 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 27.6421 – 3.4249×10^3/(T/K) –6.5804·log (T/K) + 9.3417×10^{-10}·(T/K) + 1.0547×10^{-6}·(T/K)^2; temp range 309–660 K (vapor pressure eq., Yaws 1994)
95.44* (25.35°C, transpiration method, measured range 278.3–313.7 K, Krasnykh et al. 2002)
ln (P/Pa) = (305.859/R) – [79968.084/R(T/K)] – (88.80/R)·ln[(T/K)/298.15]; temp range 278–313.7 K (transpiration method, Krasnykh et al. 2002)

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
2.64 (calculated-f const. as per Rekker 1977, Hanai et al. 1981)
2.16 (Wang et al. 1987)
2.16 (recommended, Sangster 1993)

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 $t_{½} < 0.24$ h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.3.16.1
Reported vapor pressures of benzyl ethyl ether 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·log (T/K)	(4)		

Stull 1947		Krasnykh et al. 2002			
summary of lit. data		transpiration method			
t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
26	133	278.3	19.44	298.6	95.44
52	666.6	278.7	19.59	300.1	105.16
65	1333	283.8	30.11	302.3	117.65
79.6	2666	285.1	35.31	303.2	128.09
95.4	5333	288.8	44.78	303.6	135.21
105.5	7999	290.2	52.97	307.4	177.63
118.9	13332	292.6	61.54	308.4	188.48
139.6	26664	293.7	65.53	310.2	223.55
161.5	53329	295.2	77.81	312.2	244.83
185	101325	297.3	88.33	313.7	259.37

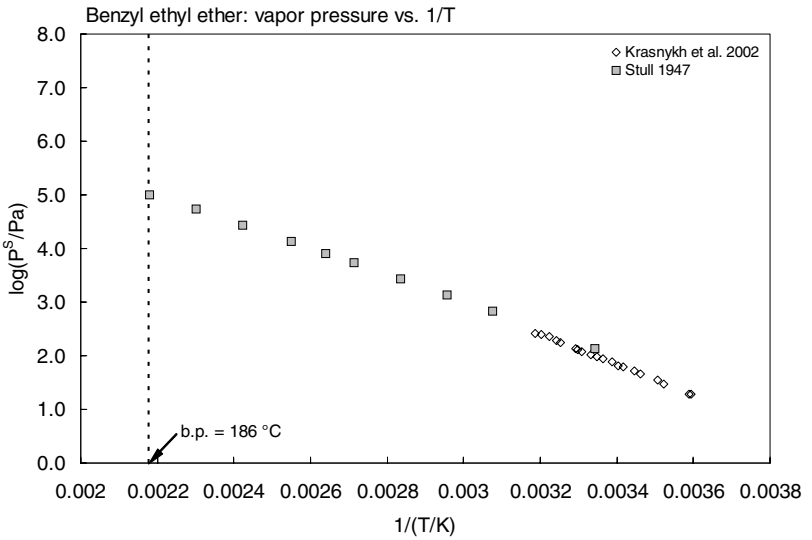
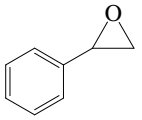


FIGURE 10.1.3.16.1 Logarithm of vapor pressure versus reciprocal temperature for benzyl ethyl ether.

10.1.3.17 Styrene oxide



Common Name: Styrene oxide
Synonym: (1,2-epoxyethyl)benzene, phenylepoxyethane
Chemical Name: (1,2-epoxyethyl)benzene, phenylepoxyethane, styrene oxide
CAS Registry No: 96-09-3
Molecular Formula: C_8H_8O
Molecular Weight: 120.149
Melting Point (°C):
–35.6 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
194.1 (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.0523 (16°C, Weast 1982–83; Dean 1985)
1.0500 (Verschueren 1983)
Molar Volume (cm^3/mol):
114.4 (20°C, calculated-density)
136.1 (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):
2800 (quoted, Verschueren 1983)
3020; 4570 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C):
40.0 (Verschueren 1983)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
1.84 (shake flask-HPLC, Pratesi et al. 1979)
1.51 (shake flask-GC, Serrentino et al. 1983)
1.61 (shake flask, Log P Database, Hansch & Leo 1987)
1.43 (Deneer et al. 1988)
1.61 (recommended, Sangster 1989, 1993)
1.51 (pH 7.5, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: $t_{½}$ = 12.3–123 h, based on estimated photooxidation rate constant with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: rate constants $k = (434 \pm 12) \times 10^{-8}$ s^{-1} at pH 7.25 and $k = (1690 \pm 620) \times 10^{-8}$ s^{-1} at pH 7.3 in sediment pores both at 25°C for water containing 0.1% w/w CH_2O as sterilant with 1-phenyl-1,2-ethanediol as major hydrolyzed product (Haag & Mill 1988);

$t_{½}$ = 0.00385–27.5 h, based on an estimation from measured first-order rate constants at 25°C, the hydrolysis half-lives at pH 5, 7 and 9 are 0.00385, 21.4 and 27.5 h (Haag & Mill 1988; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{½}$ = 24–168 h, based on biological screening test data (Schmidt-Bleek et al. 1982; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 96–672 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 $t_{½}$ < 0.24 h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976);

$t_{½}$ = 12.3–123 h, based on estimated photooxidation rate constant with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 0.00385–27.5 h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

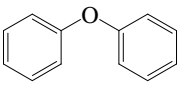
Ground water: $t_{½}$ = 0.00385–27.5 h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 0.00385–27.5 h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

Biota:

10.1.3.18 Diphenyl ether



Common Name: Diphenyl ether
Synonym: phenyl ether, diphenyl oxide, phenyl ether, 1,1′-oxybisbenzene, phenoxybenzene
Chemical Name: diphenyl ether, diphenyloxide, phenylether, phenoxybenzene
CAS Registry No: 101-84-8
Molecular Formula: $C_{12}H_{10}O$, $(C_6H_5)_2O$
Molecular Weight: 170.206
Melting Point (°C):
26.87 (Lide 2003)
Boiling Point (°C):
258 (Lide 2003)
Density (g/cm^3 at 20°C):
1.0748 (Weast 1982–83)
Molar Volume (cm^3/mol):
158.6 (20°C, calculated-density)
166.6 (Ruelle & Kesselring 1997)
195.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.217 (quoted, Riddick et al. 1986)
16.16 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.923 (mp 28.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
4000 (shake flask-residue-volume, Booth & Everson 1948)
18.7 (shake flask-UV, Vesala 1974)
18.0 (shake flask-HPLC, Banerjee et al. 1980; Pearlman et al. 1984)
21.0 (Verschueren 1983)
18, 3900 (quoted values, Riddick et al. 1986)
46.88 (supercooled liquid S_L, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

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* (66.1°C, summary of literature data, temp range 66.1–258.5°C, Stull 1947)
10.01* (40°C, dynamic method, measured range 40–60°C, Bent & Francel 1948)
log (P/mmHg) = 9.6842 – 3351.9/(t/°C + 273.1); measured range 40–60°C (dynamic method-gas saturation, Bent & Francel 1948)
log (P/mmHg) = 7.65339 – 2330.5/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
26555* (204.213°C, ebulliometry, measured range 204.2–270.9°C, Collerson et al. 1965)
log (P/mmHg) = 7.06376 – 1261.455/(221.982 + t/°C); temp range 204.2–270.9°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = 19.48322 – 2328.0/(T/K) – 3.92657·log (T/K); temp range 204.2–270.9°C (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = [–0.2185 × 12325.5/(T/K)] + 7.955679; temp range 66.1–258.5°C (Antoine eq., Weast 1972–73)
3.0* ("recomputed" reported data, temp range 204.257–271°C, Ambrose et al. 1976)
log (P/kPa) = 6.13913 – 1802.984/{(T/K) – 95.013}; temp range 477–544 K (Antoine eq., Ambrose et al. 1976)
2.67 (Verschueren 1983)
1.82 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.01104 – 1799.712/(177.744 + t/°C); temp range 204–270°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.13606 – 1799.811/(177.756 + t/°C); temp range 204.2–271°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 7.01104 – 1799.71/(177.74 + t/°C); temp range: 204–271°C (Antoine eq., Dean 1985, 1992)
2.84 (selected, Riddick et al. 1986)
log (P/kPa) = 6.13913 – 19\02.984/(178.137 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
2.93 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 8.7109 – 3351.9/(T/K); temp range 313–333K (Antoine eq., liquid, Stephenson & Malanowski 1987)
log (P/kPa) = 6.1553 – 1800.743/(T/K – 95.275); temp range 477–544K (Antoine eq., liquid, Stephenson & Malanowski 1987)
log (P/mmHg) = $-26.9635 - 2.5909 \times 10^3/(T/K) + 16.42 \cdot \log (T/K) - 2.4334 \times 10^{-2} \cdot (T/K) + 1.0244 \times 10^{-5} \cdot (T/K)^2$; temp range 300–763 K (vapor pressure eq., Yaws 1994)
2.40 (P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa m^3/mol at 25°C):
25.1 (calculated-P/C using selected data)
8.71 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
4.21, 4.36 (shake flask values, Leo et al. 1971)
4.20 (shake flask-GC, Chiou et al. 1977)
4.25 (calculated-fragment const., Rekker 1977)
4.26 (Hansch & Leo 1979)
4.08 (shake flask-HPLC, Banerjee et al. 1980)
3.79 (estimated-HPLC/MS correlation, Burkhard et al. 1985)
4.24 (calculated-f const., Burkhard et al. 1985)
3.87 (HPLC-RT correlation, Eadsforth 1986)
4.28 (shake flask, Log P Database, Hansch & Leo 1987)
4.21 (recommended, Sangster 1989, 1993)
3.949, 4.014 (shake flask method, Brooke et al. 1990)
4.21 (recommended, Hansch et al. 1995)
3.97 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
6.42 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF:
2.29 (rainbow trout, calculated, Veith et al. 1979)
2.29; 2.89 (quoted exptl., calculated-K_{OW}, Mackay 1982)

Sorption Partition Coefficient, log K_{OC}:
3.29; 3.41 (soil, quoted exptl.; calculated-MCI χ, Meylan et al. 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:
$k_1 = 5.5\ h^{-1}$, $k_2 = 0.0275\ h^{-1}$ (trout, Hawker & Connell 1985)
$1/k_2 = 36$ h (trout, Hawker & Connell 1988)
$k_2 = 0.676\ h^{-1}$ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:
Air: disappearance $t_{½} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.3.18.1
Reported vapor pressures of diphenyl ether 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
summary of lit. data

t/°C	P/Pa
66.1	133.3
97.8	666.6
114	1333
130.8	2666
150	5333
162	7999
178.8	13332
203	26664
230.7	53329
258.5	101325
mp/°C	27

Bent & Francel 1948
dynamic method

t/°C	P/Pa
40	10.01
50	21.96
60	43.97
eq. 2	P/mmHg
A	9.5842
B	3351.9
C	273.1

ΔH_v = 64.02 kJ/mol

Dreisbach & Shrader 1949
ebulliometry

No data

Antoine eq. given by Dreisbach & Martin 1949

eq. 2	P/mmHg
A	7.65339
B	2330.5
C	230
bp/°C	258.31
mp/°C	26.9

Collerson et al. 1965
ebulliometry

t/°C	P/Pa
204.13	26555
212.102	33073
219.226	40022
225.105	46611
230.561	53482
235.186	59915
239.618	66654
243.667	73327
250.991	86741
254.089	92971
257.458	100143
260.469	106906
263.29	113569
268.939	120124
268.416	126525
270.949	133333
bp/°C	257.997

Antoine eq.

eq. 2	P/mmHg
A	7.01188
B	1800.415
C	177.826

Kirchhoff eq.

eq. 4	P/mmHg
A	24.66548
B	3897.5
C	5.30117

ΔH_v = 48.62 kJ/mol

Ambrose et al. 1976
comparative ebulliometry

t/°C	P/Pa
204.257	26555
212.15	33074
219.276	40022
225.157	46611
230.616	53481
235.242	59915
239.676	66654
243.726	73327
247.473	79956
251.052	86740
254.152	92971
257.522	100144
260.534	106906
263.355	113568
266.005	120124
268.482	126525
271.015	133332
25	3

bp	531.21 K

Antoine equation:

eq. 3	P/kPa
A	6.12913
B	1802.984
C	–95.013

Coefficients of Chebyshev eq. also given in text.

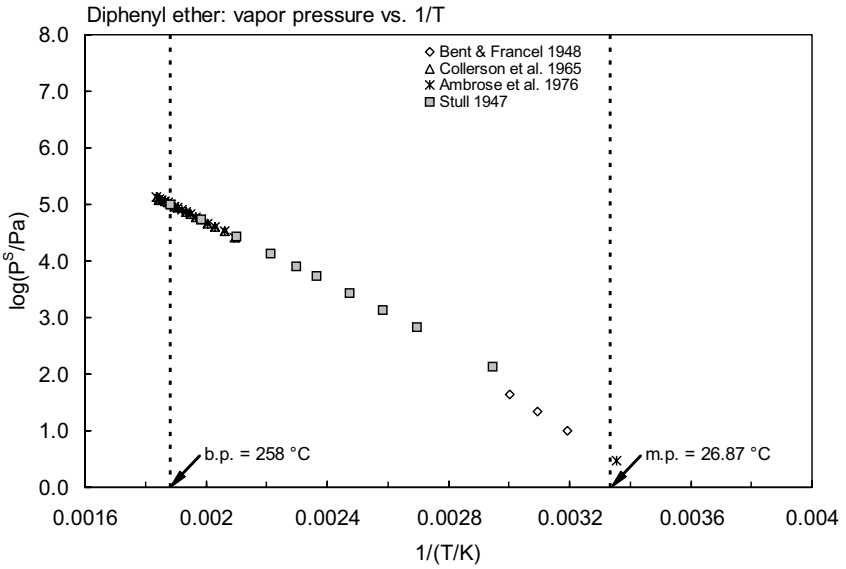
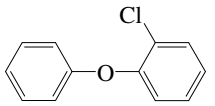


FIGURE 10.1.3.18.1 Logarithm of vapor pressure versus reciprocal temperature for diphenyl ether.

10.1.4 Polychlorinated diphenyl ethers (PCDEs)

10.1.4.1 2-Chlorodiphenyl ether (PCDE-1)



Common Name: 2-Chlorodiphenyl ether
Synonym: 2-CDPE, PCDE-1, 2-chlorobiphenyl ether
Chemical Name: 2-chlorodiphenyl ether
CAS Registry No: 2689-07-8
Molecular Formula: $C_{12}H_9ClO$
Molecular Weight: 204.652
Melting Point (°C):
45 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
216.5 (calculated-Le Bas method at normal boiling point)
179.5 (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: 0.634 (mp at 45°C)

Water Solubility (g/m^3 or mg/L at 25°C):
3.40; 4.80 (quoted exptl.; calculated-molar volume and MP, Ruelle & Kesselring 1997)
3.40 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.537 (P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol):
32.36 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
4.45 (HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
6.33 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

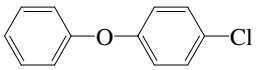
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Photolysis: photolysis rate $k_P = 0.0035\ d^{-1}$ with a half-life of 200 d in summer sunlight; $k_P(exptl) = 3.4 \times 10^{-8}\ s^{-1}$ with $t_{½}$ = 240 h, $k_P(calc) = 3.1 \times 10^{-9}\ s^{-1}$ in winter sunlight, at 40° L in surface waters (Dulin et al. 1986)

Half-Lives in the Environment:
Air:
Surface water: photolysis $t_{½}$ = 200 d in summer sunlight and $t_{½}$ = 240 d in winter sunlight at 40° L in surface waters (Dulin et al. 1986)
Ground water:
Sediment:
Soil:
Biota: $t_{½}$ = 4–63 d in trout Cl_1-DPEs to Cl_4-DPEs (Niimi et al. 1994).

10.1.4.2 4-Chlorodiphenyl ether



Common Name: 4-Chlorodiphenyl ether
Synonym: 4-chlorophenyl phenyl ether, 1-chloro-4-phenoxybenzene, p-chlorophenyl phenyl ether, 4-chlorodiphenyl ether, monochlorodiphenyl oxide
Chemical Name: 4-chlorophenyl phenyl ether, 4-chlorodiphenyl ether
CAS Registry No: 7005-72-3
Molecular Formula: $C_{12}H_9ClO$
Molecular Weight: 204.652
Melting Point (°C):
–6.0 (Callahan et al. 1979)
–8.0 (Mabey et al. 1982)
Boiling Point (°C):
284.5 (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.2026 (15°C, Weast 1982–83; Lide 2003)
Molar Volume (cm^3/mol):
216.5 (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):
3.30 (Branson 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)
59.04 (Isnard & Lambert 1988,1989)

Vapor Pressure (Pa at 25°C):
0.360 (calculated, Branson 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
22.19 (calculated-P/C, Mabey et al. 1982)
22.29 (20–25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)
24.79 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
4.08 (Branson 1977; quoted, Callahan et al. 1979; Ryan et al. 1988; Isnard & Lambert 1988,1989)
5.079 (calculated, Mabey et al. 1982)

Bioconcentration Factor, log BCF:
2.867 (rainbow trout muscle, Branson 1977; quoted, Callahan et al. 1979)
4.255 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
2.87 (quoted, Isnard & Lambert 1988)

Sorption Partition Coefficient, log K_{OC}:
4.763 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

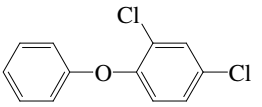
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis: photolysis rate $k_P = 0.19\ d^{-1}$ with $t_{½} = 3.6$ d in summer sunlight; $k_P(exptl) < 2.0 \times 10^{-8}\ s^{-1}$ with $t_{½} > 400$ h, $k_P(calc) = 3.7 \times 10^{-8}\ s^{-1}$ in winter sunlight, both at 40° L in surface waters (Dulin et al. 1986)
Oxidation: $k << 360\ M^{-1}\ h^{-1}$ for singlet oxygen and $k << 1.0\ M^{-1}\ h^{-1}$ for peroxy radical (Mabey et al. 1982)
Hydrolysis:

Biodegradation: $t_{½}$ = 4.0 h, measured only in activated sludge (Branson 1978; quoted, Callahan et al. 1979).
Biotransformation: estimated rate constant k = 1×10^{-7} mL $cell^{-1}$ h^{-1} for bacterial transformation in water (Mabey et al. 1982).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: photolysis $t_{½}$ = 3.6 d summer sunlight and $t_{½}$ > 400 d in winter sunlight at 40° L surface waters (Dulin et al. 1986)

10.1.4.3 2,4-Dichlorodiphenyl ether (PCDE-8)



Common Name: 2,4-Dichlorodiphenyl ether
Synonym: 2,4-DCDPE, PCDE-8
Chemical Name:
CAS Registry No: 51892-26-3
Molecular Formula: $C_{12}H_8Cl_2O$
Molecular Weight: 239.097
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
237.4 (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):
5.605 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.123 (P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
5.25 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
5.62 (Oliver & Niimi 1984)
4.93 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
7.60 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

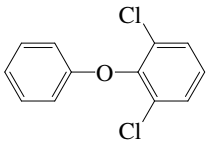
Bioconcentration Factor, log BCF or log K_B:
3.97 (rainbow trout, Oliver & Niimi 1984)

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: $t_{½}$ = 3–63 d for Cl_1-DPEs to Cl_4-DPEs in trout (Niimi et al. 1994).

10.1.4.4 2,6-Dichlorodiphenyl ether (PCDE-10)



Common Name: 2,6-Dichlorodiphenyl ether
Synonym: 2,6-DCDPE, PCDE-10
Chemical Name:
CAS Registry No: 28419-69-4
Molecular Formula: $C_{12}H_8Cl_2O$
Molecular Weight: 239.097
Melting Point (°C):
39 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
237.4 (calculated-Le Bas method at normal boiling point)
192.4 (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: 0.729 (mp at 39°C)

Water Solubility (g/m^3 or mg/L at 25°C):
2.08; 0.213 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
2.08 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.174 (supercooled liquid P_L, GC-RI correlation, Kurz & Kesselring 1997)

Henry's Law Constant (Pa·m^3/mol at 25°C):
19.95 (calculated-P/C, Kurz & Kesselring 1997)

Octanol/Water Partition Coefficient, log K_{OW}:
4.64 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
6.73 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

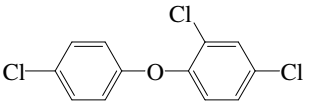
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: $t_{½}$ = 4–63 d Cl_1-DPEs to Cl_4-DPEs in trout (Niimi et al. 1994).

10.1.4.5 2,4,4′-Trichlorodiphenyl ether (PCDE-28)



Common Name: 2,4,4′-Trichlorodiphenyl ether
Synonym: 2,4,4′-TCDPE, PCDE-28
Chemical Name: 2,4,4′-trichlorodiphenyl ether
CAS Registry No: 59030-21-3
Molecular Formula: $C_{12}H_7Cl_3O$
Molecular Weight: 273.543
Melting Point (°C):
oil (Navalainen et al. 1994)
40 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
258.3 (calculated-Le Bas method at normal boiling point)
205.3 (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: 0.712 (mp at 40°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.102; 0.0385 (quoted exptl.; calculated-molar volume and mp, Ruelle & Kesselring 1997)
0.101 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.0204 (supercooled liquid P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol):
33.88 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
5.53 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
7.19 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

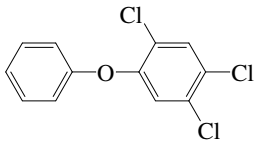
Bioconcentration Factor, log BCF or log K_B:
2.98; 3.36 (concn of 2,4,4′-trichloro-DPE 39.3; 118 μg/L, juvenile Atlantic salmon, 96-h exposure, Zitko & Carson 1977)

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: excretion $t_{½}$ = 235 h following uptake from water, excretion $t_{½}$ = 15 d following uptake from food for Juvenile salmon (Zitko & Carson 1977);
average $t_{½}$ = 15 d in salmon for trichloro-DPE congeners; biological $t_{½}$ = 63 d (range 46–104 d) in rainbow trout (average value for trichlorodiphenyl ethers (Niimi 1986);
$t_{½}$ = 4–63 d Cl_1-DPEs to Cl_4-DPEs in trout (Niimi et al. 1994).

10.1.4.6 2,4,5-Trichlorodiphenyl ether (PCDE-29)



Common Name: 2,4,5-Trichlorodiphenyl ether
Synonym: 2,4,5-TCDPE, PCDE-29
Chemical Name: 2,4,5-trichlorodiphenyl ether
CAS Registry No: 52322-80-2
Molecular Formula: $C_{12}H_7Cl_3O$
Molecular Weight: 273.543
Melting Point (°C):
oil (Opperhuizen & Voors 1987)
61 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
258.3 (calculated-Le Bas method at normal boiling point)
205.3 (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: 0.443 (mp at 61°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.050 (Opperhuizen 1986)
0.072; 0.0486 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
0.072 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.0288 (P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol):
112.2 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
5.0 (estimated, Opperhuizen 1986)
5.44 (Opperhuizen & Voors 1987; quoted, Niimi et al. 1994)
5.58 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
6.92 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:
4.18 (guppy, 8-d exposure, Opperhuizen & Voors 1987)

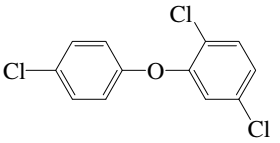
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Biotransformation: rate of metabolism k = 0.27 d^{-1} (guppy, 8-d exposure, Opperhuizen & Voors 1987)
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 > 5 \times 10^2$ d^{-1} (guppy, Opperhuizen 1986)
$k_1 = 1.5 \times 10^3$ mL g^{-1} d^{-1} (guppy, 8-d exposure, Opperhuizen & Voors 1987)
k_2 = 0.34 d^{-1} (guppy, elimination period 56 d, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: average excretion $t_{½}$ = 15 d for trichloro-DPE congeners in salmon; biological $t_{½}$ = 63 d in rainbow trout (average value for trichlorodiphenyl ethers, Niimi 1986);
$t_{½}$ = 4–63 d for Cl_1-DPEs to Cl_4-DPEs in trout (Niimi et al. 1994).

10.1.4.7 2,4′,5-Trichlorodiphenyl ether (PCDE-31)



Common Name: 2,4′,5-Trichlorodiphenyl ether
Synonym: 2,4′,5-TCDPE, PCDE-31
Chemical Name: 2,4′,5-trichlorodiphenyl ether
CAS Registry No: 65075-00-5
Molecular Formula: $C_{12}H_7Cl_3O$
Molecular Weight: 273.543
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
258.3 (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):
0.0993 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.0229 (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
6.31 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
5.66 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
5.70 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:
8.25 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

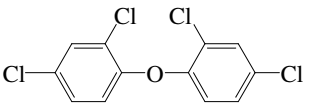
Bioconcentration Factor, log BCF or log K_B:
3.30; 2.93 (ave. concn of 2,4′,5-trichloro-DPE 2.37; 7.01 μg/L, juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: excretion $t_{½}$ = 310 h following uptake from water; $t_{½}$ = 26 d following uptake from food for juvenile Atlantic salmon (Zitko & Carson 1976);
average excretion $t_{½}$ = 15 d for trichloro-DPE congeners in salmon; biological $t_{½}$ = 63 d in rainbow trout (average value for trichlorodiphenyl ethers, Niimi 1986);
$t_{½}$ = 4–63 d Cl_1-DPEs to Cl_4-DPEs in trout (Niimi et al. 1994).

10.1.4.8 2,2′,4,4′-Tetrachlorodiphenyl ether (PCDE-47)



Common Name: 2,2′,4,4′-Tetrachlorodiphenyl ether
Synonym: 2,2′,4,4′-TCDPE, PCDE-47, 2,2′,4,4′-tetrachlorobiphenyl ether, 2.,2′,4,4′-TCBP
Chemical Name: 2,2′,4,4′-tetrachlorodiphenyl ether
CAS Registry No: 28076-73-5
Molecular Formula: $C_{12}H_6Cl_4O$
Molecular Weight: 307.988
Melting Point (°C):
69–70 (Navalainen et al. 1994)
69 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
279.2 (calculated-Le Bas method at normal boiling point)
218.2 (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: 0.366 (mp at 69.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0466; 0.0154 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
0.0466 (supercooled liquid, RP-HPLC-RI, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.00525 (P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
34.67 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
5.95 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{AO}:
7.80 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

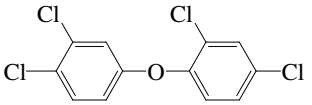
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: average excretion $t_{½}$ = 55 d in salmon for tetrachloro-DPE congeners; mean biological $t_{½}$ = 119 d (range 82–213 d) in rainbow trout (Niimi 1986);
$t_{½}$ = 4–63 d for Cl_1-DPEs to Cl_4-DPEs in trout (Niimi et al. 1994).

10.1.4.9 2,3′,4,4′-Tetrachlorodiphenyl ether (PCDE-66)



Common Name: 2,3′,4,4′-Tetrachlorodiphenyl ether
Synonym: 2,3′,4,4′-DCPE, PCDE-66
Chemical Name: 2,3′,4,4′-tetrachlorodiphenyl ether
CAS Registry No: 61328-46-9
Molecular Formula: $C_{12}H_6Cl_4O$
Molecular Weight: 307.988
Melting Point (°C):
oil (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
279.2 (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):
0.0308 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.00407 (supercooled liquid P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
40.74 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.13 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{AO}:
7.91 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmitter 1999)

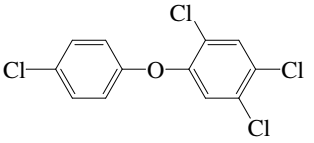
Bioconcentration Factor, log BCF or log K_B:
3.43; 3.01 (ave. concn of 2,3′,4,4′-tetrachloro-DPE 2.07; 6.03 μg/L, juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: excretion $t_{½}$ = 370 h following uptake from water, $t_{½}$ = 55 d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1976);
average excretion $t_{½}$ = 55 d in salmon for tetrachloro-DPE congeners; mean biological $t_{½}$ = 119 d (range 82–213 d) in rainbow trout (Niimi 1986);
$t_{½}$ = 4–63 d in trout for Cl_1-DPEs to Cl_4-DPEs (Niimi et al. 1994).

10.1.4.10 2,4,4′,5-Tetrachlorodiphenyl ether (PCDE-74)



Common Name: 2,4,4′,5-Tetrachlorodiphenyl ether
Synonym: 2,4,4′,5-PCDE, PCDE-74
Chemical Name: 2,4,4′,5-tetrachlorodiphenyl ether
CAS Registry No: 61328-45-8
Molecular Formula: $C_{12}H_6Cl_4O$
Molecular Weight: 307.988
Melting Point (°C):
62–63 (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
279.2 (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):
0.0281 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
4.79×10^{-3} (P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
52.48 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
5.99 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
7.66 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

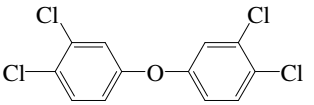
Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

Biota: average $t_{½}$ = 55 d in salmon for tetrachloro-DPE congeners (Zitko & Carson 1977; quoted, Niimi 1986); mean biological $t_{½}$ = 108 d (range 62–407 d) in rainbow trout (Niimi 1986);
$t_{½}$ = 4–63 d in trout for Cl_1-DPEs to Cl_4-DPEs; $t_{½}$ = 15 d for Cl_4-DPE to Cl_5-DPE in waterborne exposed salmon and $t_{½}$ = 55 d for diet-exposed fish (Niimi et al. 1994).

10.1.4.11 3,3′,4,4′-Tetrachlorodiphenyl ether (PCDE-77)



Common Name: 3,3′,4,4′-Tetrachlorodiphenyl ether
Synonym: 3,3′,4,4′-PCDE, PCDE-77
Chemical Name: 3,3′,4,4′-tetrachlorodiphenyl ether
CAS Registry No: 56348-72-2
Molecular Formula: $C_{12}H_6Cl_4O$
Molecular Weight: 307.988
Melting Point (°C):
- oil (Opperhuizen & Voors 1987)
- 69–71 (Navalainen et al. 1994)
- 70 (Ruelle & Kesselring 1997)

Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
- 279.2 (calculated-Le Bas method at normal boiling point)
- 218.2 (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: 0.362 (mp at 70°C)

Water Solubility (g/m^3 or mg/L at 25°C):
- 0.020 (Opperhuizen 1986)
- 0.0323; 0.00991 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
- 0.0323 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
- 2.57×10^{-3} (P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
- 24.55 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
- 6.0 (estimated, Opperhuizen 1986)
- 5.78 (Opperhuizen & Voors 1987; quoted, Niimi et al. 1994)
- 6.36 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
- 8.36 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:
- 4.50 (guppy, 8-d exposure, Opperhuizen & Voors 1987)
- 4.51; 4.09 (guppy; trout muscle, Niimi et al. 1994)
- 4.46–4.99 (calculated-$K_{OW,}$ Niimi et al. 1994)

Sorption Partition Coefficient, log K_{OC}:

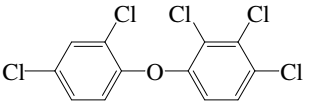
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
- $k_1 > 5 \times 10^2$ d^{-1} (Guppy, Opperhuizen 1986)

$k_1 = 9.6 \times 10^2$ mL g^{-1} d^{-1} (guppy, 8-d exposure, Opperhuizen & Voors 1987)
$k_2 = 0.03$ d^{-1} (guppy, elimination period 56 d, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: average $t_{½}$ = 55 d in salmon for tetrachloro-DPE congeners (Zitko & Carson 1977; quoted, Niimi 1986)
mean biological $t_{½}$ = 134 d (range 73–792 d) in rainbow trout (Niimi 1986);
$t_{½}$ = 23 d in guppy, $t_{½}$ = 29 d in trout muscle (Niimi et al. 1994).

10.1.4.12 2,2′,3,4,4′-Pentachlorodiphenyl ether (PCDE-85)



Common Name: 2,2′,3,4,4′-Pentachlorodiphenyl ether
Synonym: PDCE-85
Chemical Name: 2,2′,3,4,4′-pentachlorodiphenyl ether
CAS Registry No: 71585-37-0
Molecular Formula: $C_{12}H_5Cl_5O$
Molecular Weight: 342.433
Melting Point (°C):
65–67 (Navalainen et al. 1994)
66 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
300.1 (calculated-Le Bas method at normal boiling point)
231.1 (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: 0.396 (mp at 66°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0124; 0.00609 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
0.0124 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
6.92×10^{-4} (supercooled liquid P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol):
19.05 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.28 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.39 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

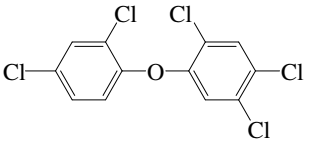
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: average $t_{½}$ = 55 d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977; Niimi 1986)
biological $t_{½}$ ~ 113 d (range 81–144 d, average value for pentachloro-DPE congeners, Niimi 1986);
$t_{½}$ = 15 d for Cl_4-DPE to Cl_5-DPE in waterborne exposed salmon and $t_{½}$ = 55 d for diet-exposed fish (Niimi et al. 1994).

10.1.4.13 2,2′,4,4′,5-Pentachlorodiphenyl ether (PCDE-99)



Common Name: 2,2′,4,4′,5-Pentachlorodiphenyl ether
Synonym: 2,2′,4,4′,5-PCDE, PCDE-99
Chemical Name: 2,2′,4,4′,5-pentachlorodiphenyl ether
CAS Registry No: 60123-64-0
Molecular Formula: $C_{12}H_5Cl_5O$
Molecular Weight: 342.433
Melting Point (°C):
oil (Navalainen et al. 1994)
25 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
300.1 (calculated-Le Bas method at normal boiling point)
231.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (calculated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
1.0 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
5.06×10^{-3}; 0.0153 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
8.406×10^{-3} (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
$\log [S_L/(mol/L)] = -1.392 - 866.2/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.35×10^{-3} (P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
1.34×10^{-3}; 1.34×10^{-3} (liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 11.90 - 4404/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 8.95 - 3525/(T/K)$ (liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
54.95 (calculated-P/C, Kurz & Ballschmiter 1999)
$\log [H/(Pa\ m^3/mol)] = 10.34 - 2659/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.38 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
7.46, 7.20 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.03 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:
3.15; 2.77 (4.01; 12.0 µg/L, ave. concn of 2,2′,4,4′,5-PCDPE (reported as 2,2′4′,5-TCDPE), juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, log K_{OC}:

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

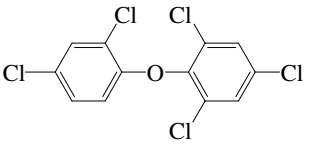
Half-Lives in the Environment:

Biota: excretion $t_{½}$ = 370 h following uptake from water, $t_{½}$ = 55 d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1977);

average excretion $t_{½}$ = 55 d in salmon for pentachloro-DPE congeners; mean biological $t_{½}$ = 144 d (range 93–311 d) in rainbow trout (Niimi 1986);

$t_{½}$ = 15 d for Cl_4-DPE to Cl_5-DPE in waterborne exposed salmon and $t_{½}$ = 55 d for diet-exposed fish (Niimi et al. 1994).

10.1.4.14 2,2′,4,4′,6-Pentachlorodiphenyl ether (PCDE-100)



Common Name: 2,2′,4,4′,6-Pentachlorodiphenyl ether
Synonym: 2,2′,4,4′,6-PCDE, PCDE-100
Chemical Name: 2,2′,4,4′,6-pentachlorodiphenyl ether
CAS Registry No: 104294-16-8
Molecular Formula: $C_{12}H_5Cl_5O$
Molecular Weight: 342.433
Melting Point (°C):
45–46 (Navalainen et al. 1994)
46 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
300.1 (calculated-Le Bas method at normal boiling point)
231.1 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (calculated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
1.0 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
0.0160 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
$\log [S_L/(mol/L)] = -1.392 - 943.0/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.19×10^{-3} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
2.17×10^{-3}; 1.34×10^{-3} (liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 11.90 - 4408/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 8.95 - 3467/(T/K)$ (liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
46.77 (calculated-P/C, Kurz & Ballschmiter 1999)
$\log [H/(Pa\ m^3/mol)] = 10.34 - 2524/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.11 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
7.11, 6.31 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
7.83 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

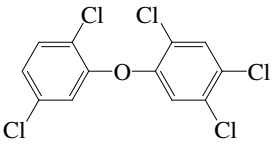
Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

Biota: excretion $t_{½}$ = 370 h following uptake from water, $t_{½}$ = 55 d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1977);
average excretion $t_{½}$ = 55 d in salmon for pentachloro-DPE congeners; mean biological $t_{½}$ = 144 d (range 93–311 d) in rainbow trout (Niimi 1986);
$t_{½}$ = 15 d for Cl_4-DPE to Cl_5-DPE in waterborne exposed salmon and $t_{½}$ = 55 d for diet-exposed fish (Niimi et al. 1994).

10.1.4.15 2,2′,4,5,5′-Pentachlorodiphenyl ether (PCDE-101)



Common Name: 2,2′,4,5,5′-Pentachlorodiphenyl ether
Synonym: PDCE-101
Chemical Name: 2,2′,4,5,5′-pentachlorodiphenyl ether
CAS Registry No: 131138-21-1
Molecular Formula: $C_{12}H_5Cl_5O$
Molecular Weight: 342.433
Melting Point (°C):
oil (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
300.1 (calculated-Le Bas method at normal boiling point)
231.1 (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

Water Solubility (g/m^3 or mg/L at 25°C):
0.00943; 0.0153 (quoted exptl.; calculated-molar volume and mp, Ruelle & Kesselring 1997)
0.00943 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
1.74×10^{-3} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol):
63.10 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.22 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
7.81 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

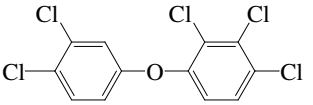
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: excretion $t_{½}$ = 370 d following uptake from water; $t_{½}$ = 55 d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1976);
average $t_{½}$ = 55 d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977; Niimi 1986);
biological $t_{½}$ = 113 d (range 81–144 d) in rainbow trout (average value of pentachloro-DPE, Niimi 1986);
$t_{½}$ = 15 d for Cl_4-DPE to Cl_5-DPE in waterborne exposed salmon and $t_{½}$ = 55 d for diet-exposed fish (Niimi et al. 1994).

10.1.4.16 2,3,3′,4,4′-Pentachlorodiphenyl ether (PCDE-105)



Common Name: 2,3,3′,4,4′-Pentachlorodiphenyl ether
Synonym: PCDE-105
Chemical Name: 2,3,3′,4,4′-pentachlorodiphenyl ether
CAS Registry No: 85918-31-6
Molecular Formula: $C_{12}H_5Cl_5O$
Molecular Weight: 324.433
Melting Point (°C):
64–66 (Navalainen et al. 1994)
65 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
300.1 (calculated-Le Bas method at normal boiling point)
231.1 (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: 0.405 (mp at 65°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.00732; 0.0059 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.00732 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
5.13×10^{-4} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
23.99 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.51 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.52 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

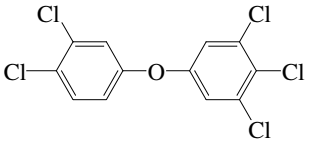
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: average $t_{½}$ = 55 d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977, Niimi 1986)
biological $t_{½}$ ~ 113 d (range 81–144 d) in rainbow trout (average value for pentachloro-DPE congeners, Niimi 1986);
$t_{½}$ = 15 d for Cl_4-DPE to Cl_5-DPE in waterborne exposed salmon and $t_{½}$ = 55 d for diet-exposed fish (Niimi et al. 1994).

10.1.4.17 3,3′,4,4′,5-Pentachlorodiphenyl ether (PCDE-126)



Common Name: 3,3′,4,4′,5-Pentachlorodiphenyl ether
Synonym: PCDE-126
Chemical Name: 3,3′,4,4′,5-pentachlorodiphenyl ether
CAS Registry No: 94339-59-0
Molecular Formula: $C_{12}H_5Cl_5O$
Molecular Weight: 342.433
Melting Point (°C):
68–70 (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
300.1 (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):
1.93×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
5.62×10^{-4} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
100 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.83 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
6.88 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:
8.22 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

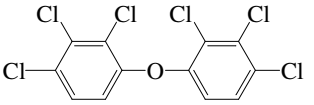
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: average $t_{½}$ = 55 d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977, Niimi 1986)
biological $t_{½}$ ~ 113 d (range 81–144 d) in rainbow trout (average value for pentachloro-DPE congeners, Niimi 1986);
$t_{½}$ = 15 d for Cl_4-DPE to Cl_5-DPE in waterborne exposed salmon and $t_{½}$ = 55 d for diet-exposed fish (Niimi et al. 1994).

10.1.4.18 2,2′,3,3′,4,4′-Hexachlorodiphenyl ether (PCDE-128)



Common Name: 2,2′,3,3′,4,4′-Hexachlorodiphenyl ether
Synonym: PCDE-128
Chemical Name: 2,2′,3,3′,4,4′-hexachlorodiphenyl ether
CAS Registry No: 71585-39-2
Molecular Formula: $C_{12}H_4Cl_6O$
Molecular Weight: 376.878
Melting Point (°C):
141–142 (Navalainen et al. 1994)
95 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
321.0 (calculated-Le Bas method at normal boiling point)
244.0 (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: 0.206 (mp at 95°C)

Water Solubility (g/m^3 or mg/L at 25°C):
2.73×10^{-3}; 4.33×10^{-4} (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
2.73×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
8.71×10^{-5} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
12.02 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.82 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
9.13 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

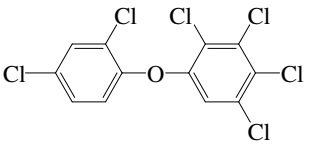
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: biological $t_{½}$ > 170 d (range 100 to > 300 d) in rainbow trout (average value for hexachloro-DPE congeners, Niimi 1986)

10.1.4.19 2,2′,3,4,4′,5-Hexachlorodiphenyl ether (PCDE-137)



Common Name: 2,2′,3,4,4′,5-Hexachlorodiphenyl ether
Synonym: PCDE-137
Chemical Name: 2,2′,3,4,4′,5-hexachlorodiphenyl ether
CAS Registry No: 71585-36-9
Molecular Formula: $C_{12}H_4Cl_6O$
Molecular Weight: 376.878
Melting Point (°C):
78–80 (Navalainen et al. 1994)
69 (Ruelle & Kesselring 1997)
80 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
321.0 (calculated-Le Bas method at normal boiling point)
244.0 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.285 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
1.85×10^{-3}; 2.18×10^{-3} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
1.61×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
$\log [S_L/(mol/L)] = -1.868 - 1043/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.0×10^{-4} (P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
2.04×10^{-4}; 5.80×10^{-5} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 12.17 - 4878/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 9.22 - 3837/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
54.95 (calculated-P/C, Kurz & Ballschmiter 1999)
$\log [H/(Pa\ m^3/mol)] = 11.09 - 2794/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.72 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
6.72, 6.83 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)
7.11 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:
8.37 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

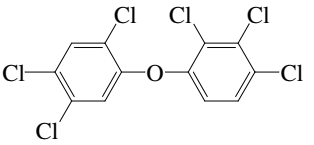
Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

Biota: mean biological $t_{½}$ = 100 d (range 69–179 d) in rainbow trout, mean $t_{½} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.20 2,2′,3,4,4′,5′-Hexachlorodiphenyl ether (PCDE-138)



Common Name: 2,2′,3,4,4′,5′-Hexachlorodiphenyl ether
Synonym: PCDE-138
Chemical Name: 2,2′,3,4,4′,5′-hexachlorodiphenyl ether
CAS Registry No: 71585-38-1
Molecular Formula: $C_{12}H_4Cl_6O$
Molecular Weight: 376.878
Melting Point (°C):
69–70 (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
321.0 (calculated-Le Bas method at normal boiling point)
244.0 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.359 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
1.84×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
log [S_L/(mol/L)] = –1.868 – 1014/(T/K) (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.70×10^{-4} (P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
1.73×10^{-4}; 6.23×10^{-5} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 12.15 – 4866/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 9.21 – 3854/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
34.67 (calculated-P/C, Kurz & Ballschmiter 1999)
log [H/(Pa m^3/mol)] = 11.08 – 2840/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
7.01 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
7.01, 6.77 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.86 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

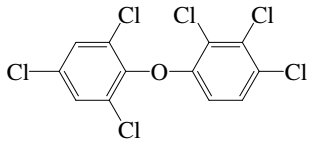
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: mean biological $t_{½}$ = 100 d (range 69–179 d) in rainbow trout; mean $t_{½}$ > 170 d (range 100 to >300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.21 2,2′,3,4,4′,6′-Hexachlorodiphenyl ether (PCDE-140)



Common Name: 2,2′,3,4,4′,6′-Hexachlorodiphenyl ether
Synonym: PCDE-140
Chemical Name: 2,2′,3,4,4′,6′-hexachlorodiphenyl ether
CAS Registry No: 106220-82-0
Molecular Formula: $C_{12}H_4Cl_6O$
Molecular Weight: 376.878
Melting Point (°C):
120–122 (Navalainen et al. 1994)
121 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
321.0 (calculated-Le Bas method at normal boiling point)
244.0 (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: 0.114 (mp at 121°C)

Water Solubility (g/m^3 or mg/L at 25°C):
2.99×10^{-3}; 6.4×10^{-4} (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
2.99×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
2.69×10^{-4} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
33.88 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.51 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

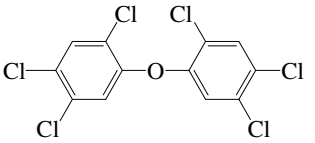
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: mean biological $t_{½}$ = 149 d (range 99–302 d) in rainbow trout; mean $t_{½}$ > 170 d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.22 2,2′,4,4′,5,5′-Hexachlorodiphenyl ether (PCDE-153)



Common Name: 2,2′,4,4′,5,5′-Hexachlorodiphenyl ether
Synonym: PCDE-153
Chemical Name: 2,2′4,4′5,5′-hexachlorodiphenyl ether
CAS Registry No: 71859-30-8
Molecular Formula: $C_{12}H_4Cl_6O$
Molecular Weight: 376.878
Melting Point (°C):
113–115 (Navalainen et al. 1994)
114 (Ruelle & Kesselring 1997)
115 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
321.0 (calculated-Le Bas method at normal boiling point)
244.0 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999))
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.134 (mp at 114°C)
0.126 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
1.65×10^{-4}; 7.52×10^{-4} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
1.65×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
$\log [S_L/(mol/L)] = -1.868 - 1047/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.47×10^{-4} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
3.74×10^{-4}; 4.71×10^{-5} (quoted supercooled liquid P_L from Hinckley et al. 1998; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 12.19 - 4916/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 9.24 - 3771/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
79.43 (calculated-P/C, Kurz & Ballschmiter 1999)
$\log (H/(Pa\ m^3/mol)) = 11.11 - 2724/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.72 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
6.72, 6.84 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.21 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

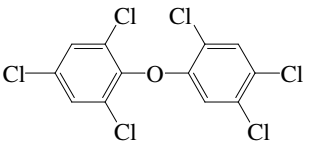
Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

Biota: mean biological $t_{½}$ = 167 d (range 98–553 d) in rainbow trout ; mean $t_{½}$ > 170 d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.23 2,2′,4,4′,5,6′-Hexachlorodiphenyl ether (PCDE-154)



Common Name: 2,2′,4,4′,5,6′-Hexachlorodiphenyl ether
Synonym: PCDE-154
Chemical Name: 2,2′,4,4′,5,6′-hexachlorodiphenyl ether
CAS Registry No: 106220-81-9
Molecular Formula: $C_{12}H_4Cl_6O$
Molecular Weight: 376.878
Melting Point (°C):
94–96 (Navalainen et al. 1994)
95 (Ruelle & Kesselring 1997)
96 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
321.0 (calculated-Le Bas method at normal boiling point)
244.0 (Ruelle & Kesselring 1997); quoted Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.206 (mp at 95°C)
0.198 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
3.44×10^{-3}; 1.16×10^{-3} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
3.44×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
$\log [S_L/(mol/L)] = -1.868 - 1090/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6.46×10^{-4} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
6.64×10^{-4}; 1.32×10^{-4} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 12.10 - 4760/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 9.15 - 4465/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
70.79 (calculated-P/C, Kurz & Ballschmiter 1999)
$\log [H/(Pa\ m^3/mol)] = 11.02 - 2582/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.49 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
6.49, 6.93 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.03 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

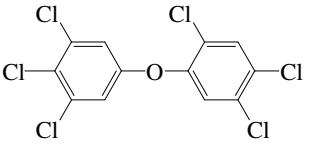
Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

Biota: mean biological $t_{½}$ = 142 d (range 90–330 d) in rainbow trout; mean $t_{½} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.24 2,3′,4,4′,5,5′-Hexachlorodiphenyl ether (PCDE-167)



Common Name: 2,3′,4,4′,5,5′-Hexachlorodiphenyl ether
Synonym: PCDE-167
Chemical Name: 2,3′,4,4′,5,5′-hexachlorodiphenyl ether
CAS Registry No: 131138-20-0
Molecular Formula: $C_{12}H_4Cl_6O$
Molecular Weight: 376.878
Melting Point (°C):
104–105 (Navalainen et al. 1994)
84 (Ruelle & Kesselring 1997)
105 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
321.0 (calculated-Le Bas method at normal boiling point)
244.0 (Ruelle & Kesselring 1997; quoted Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.161 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
7.18×10^{-4}; 1.51×10^{-3} (quoted exptl., calculated-molar volume, MP and mobile order thermodynamics, Ruelle & Kesselring 1997)
7.18×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
$\log [S_L/(mol/L)] = -1.868 - 1117/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25 and reported temperature dependence equations °C):
2.29×10^{-4} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
2.49×10^{-4}; 4.0×10^{-5} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 12.20 - 4938/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 9.25 - 3822/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
120.23 (calculated-P/C, Kurz & Ballschmiter 1997)
$\log [H/(Pa\ m^3/mol)] = 11.12 - 2705/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
7.11 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
7.11, 6.99 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.42 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

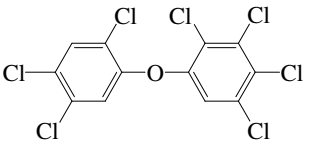
Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

Biota: mean biological $t_{½}$ > 170 d (range 100 to > 300 d) in rainbow trout for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.25 2,2′,3,4,4′,5,5′-Heptachlorodiphenyl ether (PCDE-180)



Common Name: 2,2′,3,4,4′,5,5′-Heptachlorodiphenyl ether
Synonym: PCDE-180
Chemical Name: 2,2′,3,4,4′,5,5′-heptachlorodiphenyl ether
CAS Registry No: 83992-69-2
Molecular Formula: $C_{12}H_3Cl_7O$
Molecular Weight: 411.324
Melting Point (°C):
88–90 (Navalainen et al. 1994; quoted, Passivirta et al. 1999)
89 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
341.9 (calculated-Le Bas method at normal boiling point)
256.9 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.236 (mp at 89°C)
0.227 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
1.30×10^{-4}; 4.83×10^{-4} (quoted exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
1.30×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
$\log [S_L/(mol/L)] = -2.344 - 1073/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6.31×10^{-6} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
5.14×10^{-5}; 1.17×10^{-5} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 12.31 - 5117/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 9.36 - 4046/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
199.53 (calculated-P/C, Kurz & Ballschmiter 1999)
$\log [H/(Pa\ m^3/mol)] = 11.70 - 2973/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
7.46 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
7.46, 7.20 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)
7.39 (GC-RT correlation, Hankenberg et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:
8.55 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

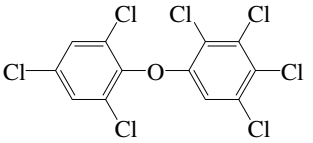
Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

Biota: mean biological $t_{½}$ = 146 d (range 90–380 d) in rainbow trout; mean $t_{½} > 300$ d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);
$t_{½}$ = 6–13 d for Cl_7-DPEs to Cl_7-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.26 2,2′,3,4,4′,5,6′-Heptachlorodiphenyl ether (PCDE-182)



Common Name: 2,2′,3,4,4′,5,6′-Heptachlorodiphenyl ether
Synonym: PCDE-182
Chemical Name: 2,2′,3,4,4′,5,6′-heptachlorodiphenyl ether
CAS Registry No: 88467-63-4
Molecular Formula: $C_{12}H_3Cl_7O$
Molecular Weight: 411.324
Melting Point (°C):
136–138 (Navalainen et al. 1994)
136 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
341.9 (calculated-Le Bas method at normal boiling point)
256.9 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.076 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
log [S_L/(mol/L)] = –2.344 – 1215/(T/K) (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.01×10^{-4}; 7.66×10^{-6} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 12.35 – 5188/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 9.49 – 3976/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol):
log [H/(Pa m^3/mol)] = 11.74 – 2761/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
7.50 (calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

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

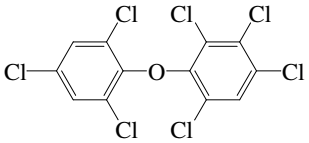
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: mean $t_{½}$ > 300 d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986); $t_{½}$ = 6–13 d for Cl_7-DPEs to Cl_9-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.27 2,2′,3,4,4′,6,6′-Heptachlorodiphenyl ether (PCDE-184)



Common Name: 2,2′,3,4,4′,6,6′-Heptachlorodiphenyl ether
Synonym: PCDE-184
Chemical Name: 2,2′,3,4,4′,6,6′-heptachlorodiphenyl ether
CAS Registry No: 106220-84-2
Molecular Formula: $C_{12}H_3Cl_7O$
Molecular Weight: 411.324
Melting Point (°C):
142 (calculated, Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
341.9 (calculated-Le Bas method at normal boiling point)
256.9 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.080 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
log [S_L/(mol/L)] = –2.344 – 1227/(T/K) (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.32×10^{-4}; 1.06×10^{-5} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 12.73 – 5858/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 9.78 – 4633/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
log [H/(Pa m^3/mol)] = 12.12 – 3406/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
7.53 (calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

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

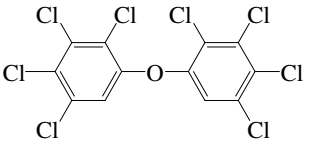
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: mean $t_{½}$ > 300 d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986); $t_{½}$ = 6–13 d for Cl_7-DPEs to Cl_9-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.28 2,2′,3,3′,4,4′,5,5′-Octachlorodiphenyl ether (PCDE-194)



Common Name: 2,2′,3,3′,4,4′,5,5′-Octachlorodiphenyl ether
Synonym: PCDE-194
Chemical Name: 2,2′,3,3′,4,4′,5,5′-octachlorodiphenyl ether
CAS Registry No:
Molecular Formula: $C_{12}H_2Cl_8O$
Molecular Weight: 445.769
Melting Point (°C):
125–128 (Navalainen et al. 1994)
126 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
362.8 (calculated-Le Bas method at normal boiling point)
269.8 (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: 0.102 (mp at 126°C)

Water Solubility (g/m^3 or mg/L at 25°C):
3.30×10^{-5}; 7.57×10^{-5} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
3.30×10^{-5} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
1.74×10^{-5} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
234.42 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
7.78 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.80 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

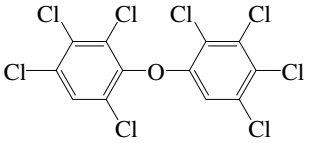
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: $t_{½}$ = 6 – 13 d for Cl_7-DPEs to Cl_9-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.29 2,2′,3,3′,4,4′,5,6′-Octachlorodiphenyl ether (PCDE-196)



Common Name: 2,2′,3,3′,4,4′,5,6′-Octachlorodiphenyl ether
Synonym: PCDE-196
Chemical Name: 2,2′,3,3′,4,4′,5,6′-octachlorodiphenyl ether
CAS Registry No: 85918-38-3
Molecular Formula: $C_{12}H_2Cl_8O$
Molecular Weight: 445.769
Melting Point (°C):
147–149 (Navalainen et al. 1994)
149 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
362.8 (calculated-Le Bas method at normal boiling point)
269.8 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0595 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
log [S_L/(mol/L)] = –2.819 – 1247/(T/K) (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.86×10^{-6}; 5.27×10^{-6} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 12.57 – 5586/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 9.62 – 4341/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
log [H/(Pa m^3/mol)] = 12.44 – 3094/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
7.88 (calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

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

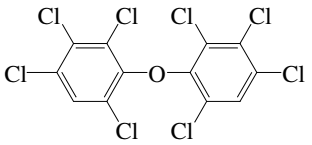
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: $t_{½}$ = 6 – 13 d for Cl_7-DPEs to Cl_9-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.30 2,2′,3,3′,4,4′,6,6′-Octachlorodiphenyl ether (PCDE-197)



Common Name: 2,2′,3,3′,4,4′,6,6′-Octachlorodiphenyl ether
Synonym: PCDE-197
Chemical Name: 2,2′,3,3′,4,4′,6,6′-octachlorodiphenyl ether
CAS Registry No: 117948-62-6
Molecular Formula: $C_{12}H_2Cl_8O$
Molecular Weight: 445.769
Melting Point (°C):
124–126 (Navalainen et al. 1994)
126 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
362.8 (calculated-Le Bas method at normal boiling point)
269.8 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.6 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.100 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
log [S_L/(mol/L)] = –2.819 – 1179/(T/K) (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.75×10^{-5}; 1.75×10^{-6} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 12.47 – 5405/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 9.52 – 4228/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):
log [H/(Pa m^3/mol)] = 12.34 – 3049/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
7.73 (calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)

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

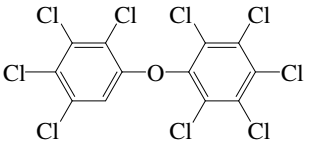
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: $t_{½}$ = 6 – 13 d for Cl_7-DPEs to Cl_9-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.31 2,2′,3,3′,4,4′,5,5′,6-Nonachlorodiphenyl ether (PCDE-206)



Common Name: 2,2′,3,3′,4,4′,5,5′,6-Nonachlorodiphenyl ether
Synonym: PCDE-206
Chemical Name: 2,2′,3,3′,4,4′,5,5′,6-nonachlorodiphenyl ether
CAS Registry No: 83992-73-8
Molecular Formula: $C_{12}HCl_9O$
Molecular Weight: 480.214
Melting Point (°C):
176–177 (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
383.7 (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):
1.704×10^{-6} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
6.92×10^{-6} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1949.84 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
8.07 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.08 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

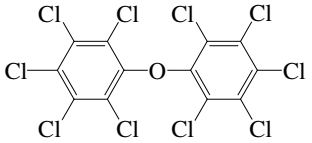
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: $t_{½}$ = 6 – 13 d for Cl_7-DPEs to Cl_9-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.32 Decachlorodiphenyl ether (PCDE-209)



Common Name: Decachlorodiphenyl ether
Synonym: PCDE-209
Chemical Name: decachlorodiphenyl ether
CAS Registry No: 31710-30-2
Molecular Formula: $C_{12}Cl_{10}O$
Molecular Weight: 514.659
Melting Point (°C):
220–222 (Navalainen et al. 1994)
131 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
404.6 (calculated-Le Bas method at normal boiling point)
295.6 (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:

Water Solubility (g/m^3 or mg/L at 25°C):
5.64×10^{-8}; 1.13×10^{-9} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
5.64×10^{-8} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
1.58×10^{-6} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):
14125 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
8.16 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
7.40 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

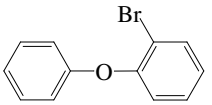
Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: mean biological $t_{½}$ = 46 d (range 27–164 d) in rainbow trout (Niimi 1986)

10.1.5 Brominated diphenyl ethers

10.1.5.1 2-Bromodiphenyl ether (BDE-1)



Common Name: 2-Bromodiphenyl ether
Synonym: BDE-1, PBDE-1, 1-bromo-2-phenoxybenzene, 2-bromophenyl phenyl ether, *o*-bromophenyl phenyl ether
Chemical Name: 2-monobromodipneyl ether
CAS Registry No: 7025-06-1
Molecular Formula: $C_{12}H_9BrO$
Molecular Weight: 249.103
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
218.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
63.7 (Wong et al. 2001)
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 and reported temperature dependence equation):
0.163; 0.163 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –3327/(T/K) + 10.37, (GC-RT correlation, Wong et al. 2001)

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}:
7.24; 7.34 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

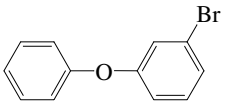
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Air: first-order degradation $t_{½}$ = 50 h (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first-order degradation $t_{½}$ = 900 h (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first-order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first-order degradation $t_{½}$ = 900 h (estimated by EPIWIN, Wania & Dugani 2003)
Biota:

10.1.5.2 3-Bromodiphenyl ether (BDE-2)



Common Name: 3-Bromodiphenyl ether
Synonym: BDE-2, PBDE-2, 1-bromo-3-phenoxybenzene, *m*-bromophenyl phenyl ether, 3-bromophenyl phenyl ether, 3-phenoxybromobenzene, 3-phenoxyphenyl bromide, *m*-bromodiphenyl ether, *m*-phenoxybromobenzene, *m*-phenoxyphenyl bromide
Chemical Name: 3-monobromodiphenyl ether
CAS Registry No: 6876-00-2
Molecular Formula: $C_{12}H_9BrO$
Molecular Weight: 249.103
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
218.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
65.4 (Wong et al. 2001)
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 and reported temperature dependence equation):
0.128; 0.125 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -3416/(T/K) + 10.56$, (GC-RT correlation, Wong et al. 2001)

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}:
7.36; 7.44 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

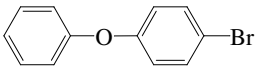
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.3 4-Bromodiphenyl ether (BDE-3)



Common Name: 4-Bromophenyl phenyl ether
Synonym: BDE-3, PBDE-3, *p*-bromophenyl phenyl ether, 1-bromo-4-phenoxybenzene, 4-bromophenyl phenyl ether, 4-phenoxybromobenzene, 4-phenoxyphenyl bromide, *p*-bromodiphenyl ether, *p*-bromophenoxybenzene, *p*-phenoxybromobenzene, *p*-phenoxyphenyl bromide
Chemical Name: 4-bromodiphenyl ether, bromophenyl ether
CAS Registry No: 101-55-3
Molecular Formula: $C_{12}H_9BrO$, C_6H_5-O-C_6H_4Br
Molecular Weight: 249.103
Melting Point (°C):
18.72 (Weast 1977, 1982–83)
18.0 (Dean 1985, 1992)
Boiling Point (°C):
310.1 (Weast 1977, 1982–83)
305 (Dean 1985, 1992)
Density (g/cm^3 at 20°C):
1.423 (Dean 1985)
Molar Volume (cm^3/mol):
154.8 (20°C, Stephenson & Malanowski 1987)
218.9 (calculated-Le Bas method at normal boiling point)
175.1 (calculated-density)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
47.9 (Tittlemier et al. 2002)
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):
4.80 (calculated-K_{OW}, Mabey et al. 1982)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.20 (20°C, calculated, Dreisbach 1952; quoted, Callahan et al. 1979; Mabey et al. 1982)
log (P_L/kPa) = 5.80633 – 1683.84/(–140.25 + T/K), temp range 463–673 K, (Antoine eq., Stephenson & Malanowski 1987)
0.259 (supercooled liquid PL, GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –2503/(T/K) + 7.81, (Clausius-Clapeyron eq. from GC-RT correlation measurement, Tittlemier et al. 2002)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
10.13 (20–25°C, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:
4.28 (calculated as per Leo et al. 1971 using data of Branson 1977, Callahan et al. 1979; quoted, Ryan et al. 1988)
4.94 (calculated, Mabey et al. 1982)
5.24 (quoted, Van Leeuwen et al. 1992)
4.85 (estimated, Tittlemier et al. 2002)

Bioconcentration Factor, log BCF:

4.114 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

4.623 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

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

Volatilization:

Photolysis:

Oxidation: << 360 M^{-1} h^{-1} for singlet oxygen and << 1.0 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982).

Hydrolysis:

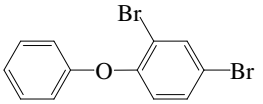
Biodegradation: estimated half-life of 4.0 h in activated sludge, based on biodegradation of 4-chlorophenyl phenyl ether in activated sewage sludge (Branson 1978; quoted, Callahan et al. 1979).

Biotransformation: estimated rate constant of 3×10^{-9} mL $cell^{-1}$ h^{-1} for the bacterial transformation in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

10.1.5.4 2,4-Dibromodiphenyl ether (BDE-7)



Common Name: 2,4-Dibromodiphenyl ether
Synonym: BDE-7, PBDE-7, 2,4-dibromo-1-phenoxybenzene
Chemical Name: 2,4-dibromodiphenyl ether
CAS Registry No: 171977-44-9
Molecular Formula: $C_{12}H_8Br_2O$
Molecular Weight: 327.999
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
242.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
75.4 (Wong et al. 2001)
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 and reported temperature dependence equation):
0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0168; 0.0153 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –3941/(T/K) + 11.34, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (for dibromodiphenyl ethers, RP-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.37; 8.36 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

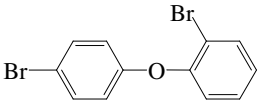
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.5 2,4′-Dibromodiphenyl ether (BDE-9)



Common Name: 2,4′-Dibromodiphenyl ether
Synonym: BDE-8, PBDE-8, 1-bromo-2-(4-bromophenoxy)-benzene
Chemical Name: 2,4′-dibromodiphenyl ether
CAS Registry No: 147217-71-8
Molecular Formula: $C_{12}H_8Br_2O$
Molecular Weight: 327.999
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
242.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
76.4 (Wong et al. 2001)
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 and reported temperature dependence equation):
0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0137; 0.0124 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –3991/(T/K) + 11.42, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.47; 8.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

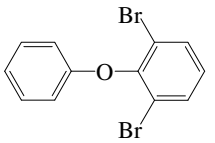
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.6 2,6-Dibromodiphenyl ether (BDE-10)



Common Name: 2,6-Dibromodiphenyl ether
Synonym: BDE-10, PBDE-10, 1,3-dibromo-2-phenoxybenzene
Chemical Name: 2,6-dibromodiphenyl ether
CAS Registry No: 51930-04-2
Molecular Formula: $C_{12}H_8Br_2O$
Molecular Weight: 327.999
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
242.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
73.1 (Wong et al. 2001)
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 and reported temperature dependence equation):
0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0277; 0.0256 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –3818/(T/K) + 11.25, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.12; 8.13 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

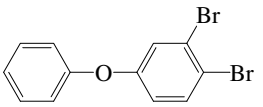
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.7 3,4-Dibromodiphenyl ether (BDE-12)



Common Name: 3,4-Dibromodiphenyl ether
Synonym: BDE-12, PBDE-12, 1,2-dibromo-4-phenoxybenzene
Chemical Name: 3,4-dibromodiphenyl ether
CAS Registry No: 189084-59-1
Molecular Formula: $C_{12}H_8Br_2O$
Molecular Weight: 327.999
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
242.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
77.4 (Wong et al. 2001)
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 and reported temperature dependence equation):
0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0119; 0.107 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4020/(T/K) + 11.56, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.55; 8.52 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

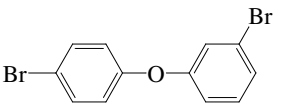
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.8 3,4′-Dibromodiphenyl ether (BDE-13)



Common Name: 3,4′-Dibromodiphenyl ether
Synonym: BDE-13, PBDE-13, 1-bromo-3-(4-bromophenoxy)-benzene
Chemical Name: 3,4′-dibromodiphenyl ether
CAS Registry No: 83694-71-7
Molecular Formula: $C_{12}H_8Br_2O$
Molecular Weight: 327.999
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
242.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
77.0 (Wong et al. 2001)
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 and reported temperature dependence equation):
0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0113; 0.0101 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4044/(T/K) + 11.62, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.57; 8.54 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

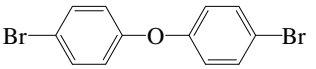
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.9 4,4′-Dibromodiphenyl ether (BDE-15)



Common Name: 4,4′-Dibromodiphenyl ether
Synonym: BDE-15, PBDE-15, 1,1-oxybis[4-bromo]benzene, bis(4-bromophenyl)ether, *p, p′*-dibromodiphenyl ether
Chemical Name: 4,4′-dibromodiphenyl ether
CAS Registry No: 2050-47-7
Molecular Formula: $C_{12}H_8Br_2O$
Molecular Weight: 327.999
Melting Point (°C):
57–58 (Tittlemier et al. 2002)
57.7 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
242.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
78.0 (Wong et al. 2001)
67.7 (Tittlemier et al. 2002)
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:
0.477 (mp at 57.5°C, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at 25°C):
0.130 (generator column-GC/ECD, Tittlemier et al. 2002)
0.273, 0.79 (supercooled S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
9.84×10^{-3}; 8.80×10^{-3} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4074/(T/K) + 11.65, (GC-RT correlation, Wong et al. 2001)
0.0173 (supercooled liquid P_L, GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –3528/(T/K) + 10.08, (Clausius-Clapeyron equation from GC-RT correlation measurements, Tittlemier et al. 2002)
0.0143, 0.010 (supercooled, P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
21 (calculated-P_L/C_L, Tittlemier et al. 2002)
4.11 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.03 (value for dibromodiphenyl ether, Pijnenburg et al. 1995)
5.55 (estimated, Tittlemier et al. 2002)
5.03, 5.48 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, log K_{OA}:
8.64; 8.60 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

8.79, 8.63 (selected measured value, final adjusted value, Wania & Dugani 2003)

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: photochemical degradation pathway of BDE15 undergoes strict debromination via first-order decay, $k = 1.98 \times 10^{-2}$ min^{-1} in 100% CH_3CN and $k = 3.10 \times 10^{-2}$ min^{-1} in CH_3OH, corresponding to $t_{½} \sim 30$ min. (Rayne et al. 2003)

Photooxidation:

Hydrolysis:

Biodegradation: complete debromination under anaerobic microbial degradation in a fixed-film plug-flow bioreactor (Rayne et al. 2003)

Biotransformation:

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

Half-Lives in the Environment:

Air: first order degradation $t_{½} = 120$ h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{½} = 1440$ h (estimated by EPIWIN, Wania & Dugani 2003)

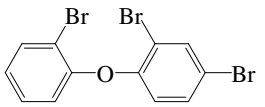
Ground water:

Sediment: first order degradation $t_{½} = 5760$ h (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{½} = 1440$ h (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

10.1.5.10 2,2′,4-Tribromodiphenyl ether (BDE-17)



Common Name: 2,2′,4-Tribromodiphenyl ether
Synonym: PBDE-17
Chemical Name: 2,2′,4-tribromodiphenyl ether
CAS Registry No: 147217-75-2
Molecular Formula: $C_{12}H_7Br_3O$
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
265.5 (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):
0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)
0.00219 (supercooled P_L, GC-RT correlation on a CPSil-8 column,Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58 (quoted range of value for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

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:
9.30* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –3.54 + 3803/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
9.966, 9.385, 8.841, 8.332 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
9.919, 9.339, 8.789, 8.290 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

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 10.1.5.10.1
Reported octanol-air partition coefficients of 2,2′,4-tribromodiphenyl ether (PBDE 17) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	9.777	15	9.966
25	9.27	25	9.385
35	8.901	35	8.841
45	8.517	45	8.332
25	9.3	QRSETP model 5	
		15	9.919
log K_{OA} = A + B/(T/K)		25	9.339
A	–3.45	35	8.798
B	3803	45	9.29
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 72.8			

Quantitative relationships between structures, environmental temperatures and properties.

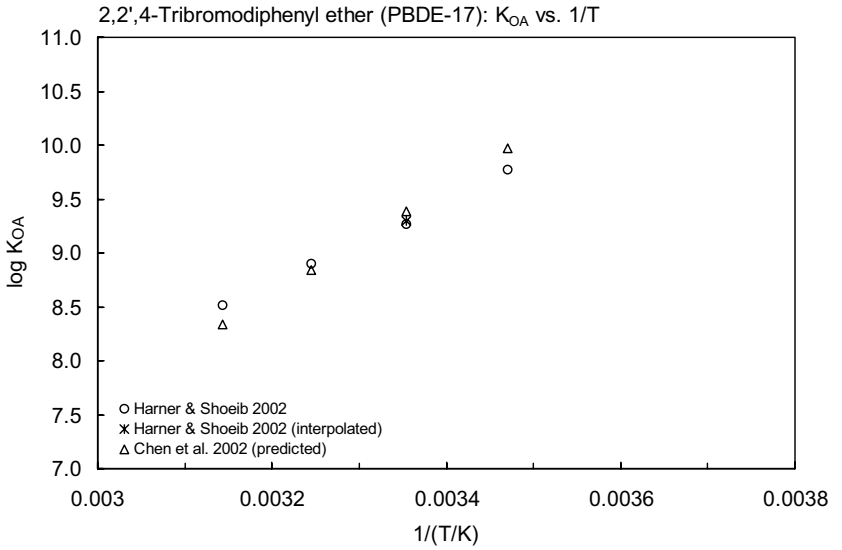
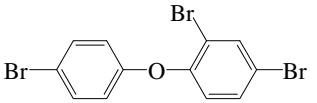


FIGURE 10.1.5.10.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2′,4-tribromodiphenyl ether (PBDE-17).

10.1.5.11 2,4,4′-Tribromodiphenyl ether (BDE-28)



Common Name: 2,4,4′-Tribromodiphenyl ether
Synonym: PBDE-28, 2,4-dibromo-1-(4-bromophenoxy)-benzene, p=bromophenyl 2,4-dibromophenyl ether
Chemical Name: 2,4,4′-tribromodiphenyl ether
CAS Registry No: 41318-75-6
Molecular Formula: $C_{12}H_7Br_3O$
Molecular Weight: 406.895
Melting Point (°C):
64–64.5 (Tittlemier et al. 2002)
64.25 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
94.05 (Tittlemier & Tomy 2001)
79.7 (Tittlemier et al. 2002)
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:
0.409 (at mp 64.25°C, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at 25°C):
0.00038 (calculated for triBDE, Alcock et al. 1999)
0.070 (solid S_S, generator column-GC/ECD, Tittlemier et al. 2002)
0.173, 0.334 (supercooled liquid S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)
1.78×10^{-4} (supercooled liquid P_L: GC-RT correlation, Tittlemier & Tomy 2001)
$\log (P_L/Pa) = -4912/(T/K) + 12.73$, (GC-RT correlation, Tittlemier & Tomy 2001)
0.00160 (supercooled P_L, GC-RT correlation on a CPSil-8 column, Wong et al. 2001)
2.19×10^{-3} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
$\log (P_L/Pa) = -4160/(T/K) + 11.30$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
1.96×10^{-3}, 1.57×10^{-3} (supercooled P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
5.1 (calculated-P_L/C_L, Tittlemier et al. 2002)
1.924 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58 (values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)
5.98 (estimated from PCDEs and fragment constant, Tittlemier et al. 2002)
5.53, 5.80 (selected measured value, final adjusted value, Wania & Dugani 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:
9.50* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –3.54 + 3889/(T/K), temp range 15–45°C (generator column-GC, Harner & Shoeib 2002)
10.279, 9.689, 9.154, 8.645 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
10.213, 9.634, 9.902, 8.585 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
9.50, 9.41 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.019 d^{-1} with $t_{½}$ = 36.5 d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:
Air: first order degradation $t_{½}$ = 128 h (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first order degradation $t_{½}$ = 1440 h (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first order degradation $t_{½}$ = 5760 h (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first order degradation $t_{½}$ = 1440 h (estimated by EPIWIN, Wania & Dugani 2003)
Biota: depuration $t_{½}$ = 36.5 d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.11.1
Reported octanol-air partition coefficients of 2,4,4′-tribromodiphenyl ether (PBDE 28) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	9.994	15	10.279
25	9.46	25	9.698
35	9.077	35	9.154
45	8.709	45	8.645
25	9.5	QRSETP model 5	
		15	10.213
log K_{OA} = A + B/(T/K)		25	9.634
A	–3.54	35	9.092
B	3889	45	8.585
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 74.5			

Quantitative relationships between structures, environmental temperatures and properties.

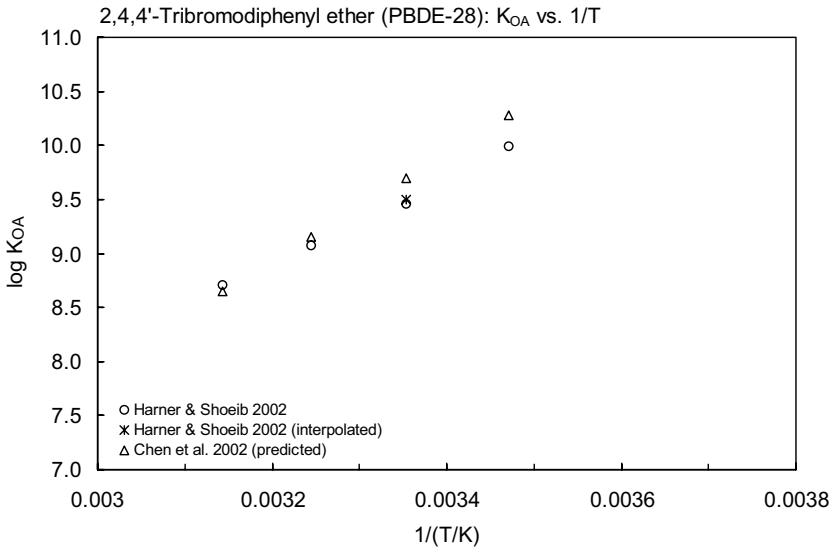
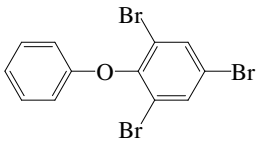


FIGURE 10.1.5.11.1 Logarithm of K_{OA} versus reciprocal temperature for 2,4,4′-tribromodiphenyl ether (PBDE-28).

10.1.5.12 2,4,6-Tribromodiphenyl ether (BDE-30)



Common Name: 2,4,6-Tribromodiphenyl ether
Synonym: PBDE-30, BDE-30, 1,3,5-tribromo-2-phenoxybenzene
Chemical Name: 2,4,6-tribromodiphenyl ether
CAS Registry No: 155999-95-4
Molecular Formula: $C_{12}H_7Br_3O$
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
85.1 (Wong et al. 2001)
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):
0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00150 (estimated for triBDE, Alcock et al. 1999)
4.56×10^{-3}; 3.96×10^{-3} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -4232/(T/K) + 11.85$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.47–5.58 (tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58 (quoted values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
9.02; 8.94 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

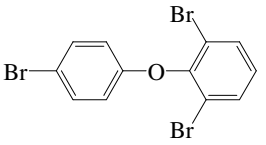
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.13 2,4′,6-Tribromodiphenyl ether (BDE-32)



Common Name: 2,4′,6-Tribromodiphenyl ether
Synonym: PBDE-32, BDE-32, 1,3-dibromo-2-(4-bromophenoxy)-benzene
Chemical Name: 2,4′,6-tribromodiphenyl ether
CAS Registry No: 189083-60-4
Molecular Formula: $C_{12}H_7Br_3O$
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
83.3 (Wong et al. 2001)
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):
0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00150 (estimated for triBDE, Alcock et al. 1999)
2.25×10^{-3}; 1.90×10^{-3} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -4352/(T/K) + 11.94$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.59 (quoted values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
9.28; 9.18 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

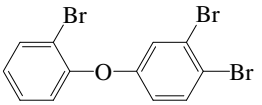
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.14 2′,3,4-Tribromodiphenyl ether (BDE-33)



Common Name: 2′,3,4-Tribromodiphenyl ether
Synonym: PBDE-33, BDE-33. 1,2-dibromo-4-(2-bromophenoxyl)-benzene
Chemical Name: 2′,3,4-tribromodiphenyl ether
CAS Registry No: 147217-78-5
Molecular Formula: $C_{12}H_7Br_3O$
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
81.0 (Wong et al. 2001)
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):
0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.01150 (estimated for tri-BDE, Alcock et al. 1999)
1.78×10^{-3}; 1.49×10^{-3} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -4443/(T/K) + 12.15$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58 (quoted range of values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

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

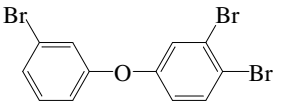
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.15 3,3′,4-Tribromodiphenyl ether (BDE-35)



Common Name: 3,3′,4-Tribromodiphenyl ether
Synonym: PBDE-35, BDE-35, 1,2-dibromo-4-(4-bromophenoxy)-benzene
Chemical Name: 3,3′,4-tribromodiphenyl ether
CAS Registry No: 147217-80-9
Molecular Formula: $C_{12}H_7Br_3O$
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
86.4 (Wong et al. 2001)
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):
0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00155 (estimated for triBDE, Alcock et al. 1999)
1.39×10^{-3}; 1.15×10^{-3} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -4512/(T/K) + 12.28$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58 (quoted range of values for tribromodiphenyl ethers, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
9.61; 9.48 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

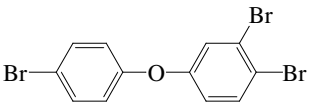
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.16 3,4,4′-Tribromodiphenyl ether (BDE-37)



Common Name: 3,4,4′-Tribromodiphenyl ether
Synonym: PBDE-37, BDE-37, 1,2-dibromo-4-(4-bromophenoxy)-benzene
Chemical Name: 3,4,4′-tribromodiphenyl ether
CAS Registry No: 147217-81-0
Molecular Formula: $C_{12}H_7Br_3O$
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
86.7 (Wong et al. 2001)
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):
0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)
1.02×10^{-3}; 8.0×10^{-4} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -4528/(T/K) + 12.20$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58 (quoted range of values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
9.68; 9.54 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

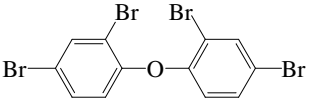
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.17 2,2′,4,4′-Tetrabromodiphenyl ether (BDE-47)



Common Name: 2,2′,4,4′-Tetrabromodiphenyl ether
Synonym: PBDE-47, BDE-47, 1,1¢-oxybis[2,4-dibromo-benzene], NSC 21724
Chemical Name: 2,2′,4,4′-tetrabromodiphenyl ether
CAS Registry No: 5436-43-1
Molecular Formula: $C_{12}H_6Br_4O$
Molecular Weight: 485.791
Melting Point (°C):
83.5–84.5 (Tittlemier et al. 2002)
84.0 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
288.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
103.13 (Tittlemier & Tomy 2001)
92.0 (Wong et al. 2001)
94.6 (Tittlemier et al. 2002)
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:
0.261 (calculated at mp 84°C, Wania & Dugani 2002)

Water Solubility (g/m^3 or mg/L at 25°C):
0.00007 (calculated for tetra-BDE, Alcock et al. 1999)
0.015 (solid S_S, generator column-GC/ECD, Tittlemier et al. 2002)
0.0496, 0.0947 (supercooled liquid S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
3.35×10^{-4}–2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
2.19×10^{-5} (supercooled liquid P_L: GC-RT correlation, Tittlemier & Tomy 2001)
$\log (P_L/Pa) = -5386/(T/K) + 13.42$, (GC-RT correlation, Tittlemier & Tomy 2001)
3.19×10^{-4}; 2.50×10^{-4} (supercooled P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -4805/(T/K) + 12.62$, (GC-RT correlation, Wong et al. 2001)
1.86×10^{-4} (supercooled liquid P_L, GC-RT correlation, Tittlemier et al. 2002)
$\log (P_L/Pa) = -4940/(T/K) + 12.85$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
2.66×10^{-4}, 2.15×10^{-4} (supercooled P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.5 (calculated-P/C, Tittlemier et al. 2002)
1.107 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
6.02 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)
6.55 (estimated, Tittlemier et al. 2002)
6.11, 6.39 (selected measured value, final adjusted value, Wania & Dugani 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:

10.53* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –6.47 + 5068/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
10.987, 10.406, 9.863, 9.353 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
10.928, 10.349, 9.807, 9.300 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
10.34; 10.14 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
10.53, 10.44 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

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

k_1 = 120 L d^{-1} g^{-1} dry wt, k_2 = 0.090 d^{-1} in blue mussels (Gustafsson et al. 1999)
k_1 = 0.108 g org. C g^{-1} lipid h^{-1} in Lake Höytiäinen sediment; 0.251 g org. C g^{-1} lipid h^{-1} in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)
k_2 = 0.034 d^{-1} in Lake Höytiäinen sediment; 0.071 d^{-1} in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)
k_2 = 0.023 d^{-1} with $t_{½}$ = 30.1 d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

Air: first order degradation $t_{½}$ = 256 h (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first order degradation $t_{½}$ = 14400 h (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Biota: depuration half-life of 7.7 d in blue mussels (Gustafsson et al. 1999);
biphasic depuration kinetics observed in oligochaete tissues with half-life of 10.5–47.5 h in compartment A for sediment ingesting obliochaetes (Leppänen & Kukkonen 2004)
depuration $t_{½}$ = 30.1 d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.17.1
Reported octanol-air partition coefficients of 2,2′,4,4′-tetrabromodiphenyl ether (PBDE 47) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	11.129	15	10.987
25	10.499	25	10.406
35	10.063	35	9.863
45	9.428	45	9.353
25	10.53	QRSETP model 5	
		15	10.928
log K_{OA} = A + B/(T/K)		25	10.349
A	–6.47	35	9.807
B	5068	45	9.3
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 97.0			

Quantitative relationships between structures, environmental temperatures and properties.

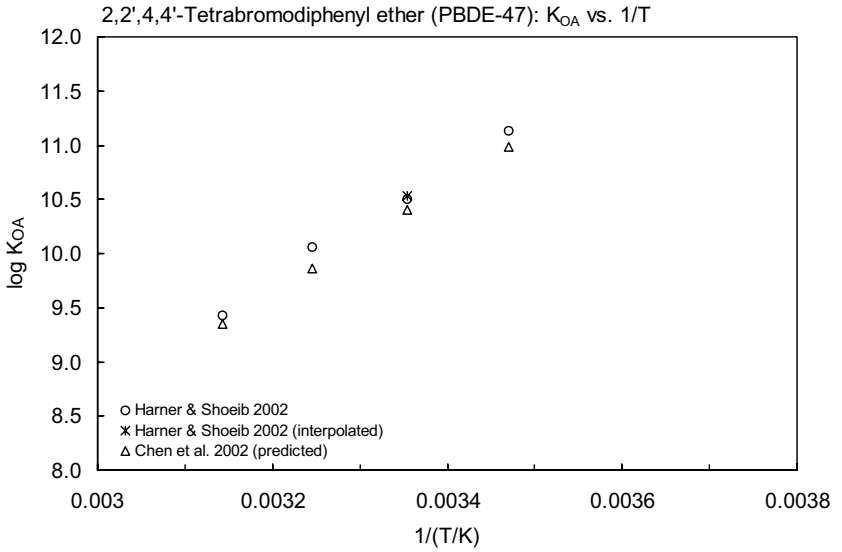
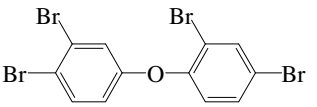


FIGURE 10.1.5.17.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2′,4,4′-tetrabromodiphenyl ether (PBDE-47).

10.1.5.18 2,3′,4,4′-Tetrabromodiphenyl ether (BDE-66)



Common Name: 2,3′,4,4′-Tetrabromodiphenyl ether
Synonym: PBDE-66, BDE-66, 1,2-dibromo-4-(2,4-dibromophenoxy)-benzene
Chemical Name: 2,3′,4,4′-tetrabromodiphenyl ether
CAS Registry No: 189084-61-5
Molecular Formula: $C_{12}H_6Br_4O$
Molecular Weight: 485.791
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
288.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
93.5 (Wong et al. 2001)
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):
0.00007 (calculated for tetraBDE, Alcock et al. 1999)
0.018 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
3.35×10^{-4}–2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
2.38×10^{-4}; 1.90×10^{-4} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4882/(T/K) + 12.75, (GC-RT correlation, Wong et al. 2001)
1.22×10^{-4} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –5109/(T/K) + 13.23, (Clausius-Clapeyron eq. form GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.50 (calculated-P_L/C_L, Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
6.73 (estimated, Tittlemier et al. 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:
10.82* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –7.88 + 5576/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
11.348, 10.767, 10.223, 9.714 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
11.281, 10.702, 10.161, 9.653 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
10.49; 10.28 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

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 10.1.5.18.1
Reported octanol-air partition coefficients of 2,3′,4,4′-tetrabromodiphenyl ether (PBDE 66) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	11.516	15	11.348
25	10.773	25	10.767
35	10.224	35	10.223
45	9.673	45	9.714
25	10.82	QRSETP model 5	
		15	11.281
log K_{OA} = A + B/(T/K)		25	10.702
A	–7.88	35	10.161
B	5576	45	9.653
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 107.0			

Quantitative relationships between structures, environmental temperatures and properties.

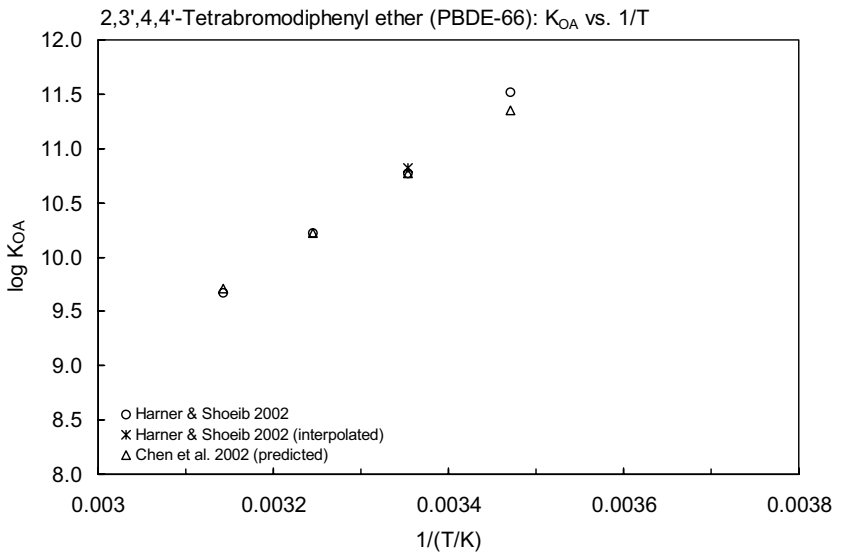
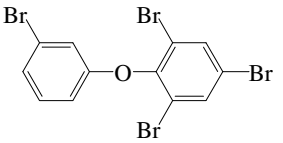


FIGURE 10.1.5.18.1 Logarithm of K_{OA} versus reciprocal temperature for 2,3′,4,4′-tetrabromodiphenyl ether (PBDE-66).

10.1.5.19 2,3′,4,6-Tetrabromodiphenyl ether (BDE-69)



Common Name: 2,3′,4,6-Tetrabromodiphenyl ether
Synonym: PBDE-69, BDE-69, 1,3,5-tribromo-2-(30bromophenoxy)-benzene
Chemical Name: 2,3′,4,6-tetrabromodiphenyl ether
CAS Registry No: 327185-09-1
Molecular Formula: $C_{12}H_6Br_4O$
Molecular Weight: 485.791
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
288.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
91.1 (Wong et al. 2001)
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):
0.00007 (calculated for tetraBDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
3.35×10^{-4}–2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
4.0×10^{-4}; 3.20×10^{-4} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -4757/(T/K) + 12.56$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
10.23; 10.04 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

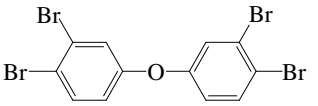
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.20 3,3′,4,4′-Tetrabromodiphenyl ether (BDE-77)



Common Name: 3,3′,4,4′-Tetrabromodiphenyl ether
Synonym: PBDE-77, BDE-77, 1,1′-xylbix[2,3-dibromophenoxy]-benzene
Chemical Name: 3.3′,4,4′-tetrabromodiphenyl ether
CAS Registry No: 93703-48-1
Molecular Formula: $C_{12}H_6Br_4O$
Molecular Weight: 485.791
Melting Point (°C):
96.7–98 (Tittlemier et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
288.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
95.3 (Wong et al. 2001)
98.7 (Tittlemier et al. 2002)
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):
0.00007 (calculated for tetraBDE, Alcock et al. 1999)
0.006 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
3.35×10^{-4}–2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
1.56×10^{-4}; 1.20×10^{-4} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4977/(T/K) + 12.89, (GC-RT correlation, Wong et al. 2001)
6.79×10^{-5} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –5156/(T/K) + 13.13, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.2 (calculated-P_L/C_L, Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
6.96 (estimated, Tittlemier et al. 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:
10.87* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –5.69 + 4936/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
11.343, 10.762, 10.218, 9.709 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
11.218, 10.603, 10.097, 9.590 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
10.70; 10.46 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

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 10.1.5.20.1
Reported octanol-air partition coefficients of 3,3′,4,4′-tetrabromodiphenyl ether (PBDE 77) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	11.486	15	11.343
25	10.829	25	10.762
35	10.371	35	10.218
45	9.844	45	9.709
25	10.87	QRSETP model 5	
		15	11.218
log K_{OA} = A + B/(T/K)		25	10.639
A	–5.69	35	10.097
B	4936	45	9.59
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 94.5			

Quantitative relationships between structures, environmental temperatures and properties.

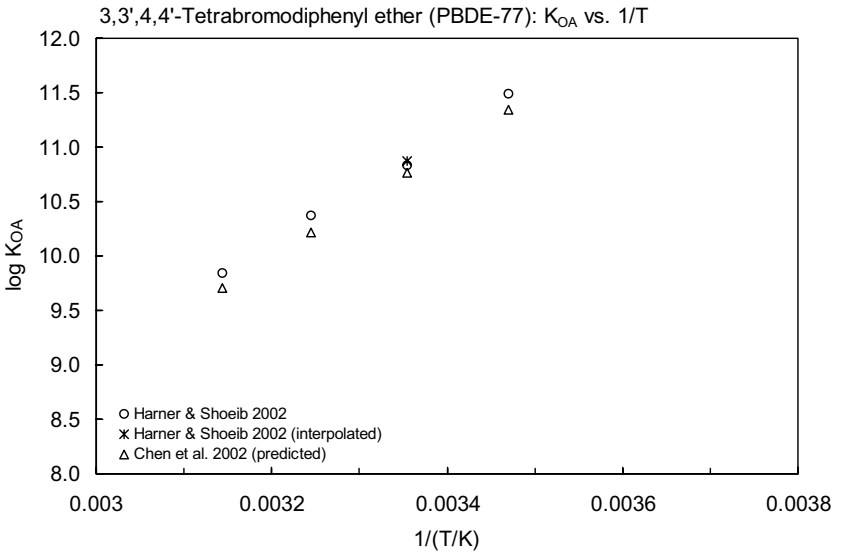
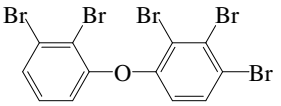


FIGURE 10.1.5.20.1 Logarithm of K_{OA} versus reciprocal temperature for 3,3′,4,4′-tetrabromodiphenyl ether (PBDE-77).

10.1.5.21 2,2′,3,3′,4-Pentabromodiphenyl ether (BDE-82)



Common Name: 2,2′,3,3′,4-Pentabromodiphenyl ether
Synonym: PBDE-82, BDE-82, 1,2,3-tribromo-4-(2,3-dibromophenoxy)-benzene
Chemical Name: 2,2′,3,3′,4-pentabromodiphenyl ether
CAS Registry No: 327185-11-5
Molecular Formula: $C_{12}H_5Br_5O$
Molecular Weight: 564.687
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
312.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
99.1 (Wong et al. 2001)
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):
6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
7.33×10^{-5}–1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.07 (estimated for pentaBDE, Alcock et al. 1999)
6.47×10^{-5}; 4.80×10^{-5} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -5175/(T/K) + 13.12$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
11.14; 10.86 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

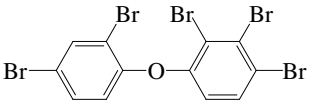
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.22 2,2′,3,4,4′-Pentabromodiphenyl ether (BDE-85)



Common Name: 2,2′,3,4,4′-Pentabromodiphenyl ether
Synonym: PBDE-85, BDE-85, 1,2,3-tribromo-4-(2,4-dibromophenoxy)-benzene
Chemical Name: 2,2′,3,3,4,4′-pentabromodiphenyl ether
CAS Registry No: 182346-21-0
Molecular Formula: $C_{12}H_5Br_5O$
Molecular Weight: 564.687
Melting Point (°C):
119–121 (Tittlemier et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
312.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
110.95 (Tittlemier & Tomy 2001)
110 (Tittlemier et al. 2002)
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):
6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)
0.006 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
7.33×10^{-5}–1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.07 (estimated for pentaBDE, Alcock et al. 1999)
2.88×10^{-6} (supercooled liquid P_L: GC-RT correlation, Tittlemier & Tomy 2001)
$\log (P_L/Pa) = -5795/(T/K) + 13.91$, (GC-RT correlation, Tittlemier & Tomy 2001)
2.81×10^{-5} (supercooled P_L, GC-RT correlation on a CPSil-8 column, Wong et al. 2001)
9.86×10^{-6} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
$\log (P_L/Pa) = -5761/(T/K) + 14.43$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.11 (calculated-P_L/C_L, Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
7.03 (estimated, Tittlemier et al. 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:
11.66* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
12,312, 11.631, 11.118, 10.544 (15, 25, 35, 45°C, generator column-GC/MS, Harner & Shoeib 2002)
$\log K_{OA} = -6.22 + 5331/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
12.131, 11.549, 11.006, 10.497 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
12.130, 11.551, 11.009, 10.502 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

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 10.1.5.22.1
Reported octanol-air partition coefficients of 2,2′,3,4,4′-pentabromodiphenyl ether (PBDE 85) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	12.312	15	12.131
25	11.631	25	11.549
35	11.118	35	11.006
45	10.544	45	10.497
25	11.66	QRSETP model 5	
		15	12.13
log K_{OA} = A + B/(T/K)		25	11.551
A	–6.22	35	11.009
B	5331	45	10.502
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 102.0			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

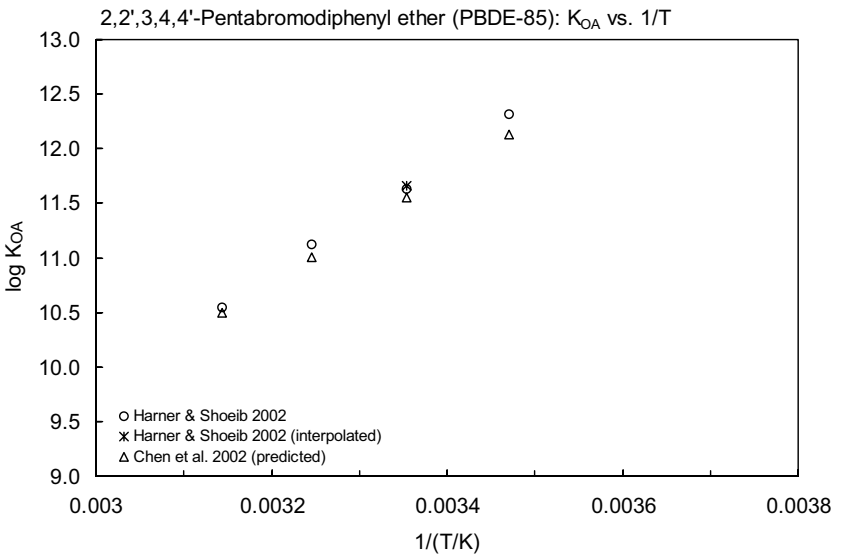
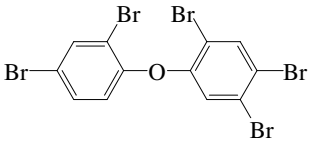


FIGURE 10.1.5.22.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2′,3,4,4′-pentabromodiphenyl ether (PBDE-85).

10.1.5.23 2,2′,4,4′,5-Pentabromodiphenyl ether (BDE-99)



Common Name: 2,2′,4,4′,5-Pentabromodiphenyl ether
Synonym: PBDE-99, BDE-99, 1,2,4-tribromo-5-(2,4-dibromophenoxy)-benzene
Chemical Name: 2,2′,4,4′,5-pentabromodiphenyl ether
CAS Registry No: 60348-60-9
Molecular Formula: $C_{12}H_5Br_5O$
Molecular Weight: 564.687
Melting Point (°C):
90.5–94.5 (Tittlemier et al. 2002)
92.5 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
312.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
104.80 (Tittlemier & Tomy 2001)
100.2 (Wong et al. 2001)
108 (Tittlemier et al. 2002)
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:
0.215 (at mp 92.5°C, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at 25°C):
6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)
0.0094 (solid S_S, generator column-GC/ECD, Tittlemier et al. 2002)
0.0275, 0.0389 (supercooled S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
7.33×10^{-5}–1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.07 (estimated for pentaBDE, Alcock et al. 1999)
1.26×10^{-5} (supercooled liquid P_L: GC-RT correlation, Tittlemier & Tomy 2001)
$\log (P_L/Pa) = -5474/(T/K) + 13.47$, (GC-RT correlation, Tittlemier & Tomy 2001)
6.82×10^{-5}; 5.0×10^{-5} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -5241/(T/K) + 13.41$, (GC-RT correlation, Wong et al. 2001)
1.76×10^{-5} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
$\log (P_L/Pa) = -5339/(T/K) + 13.37$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
4.57×10^{-5}, 3.63×10^{-5} (supercooled P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.23 (calculated-P_L/C_L, Tittlemier et al. 2002)
0.530 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.81 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)
7.13 (estimated, Tittlemier et al. 2002)
6.61, 6.76 (selected measured value, final adjusted value, Wania & Dugani 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:

11.31* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –4.64 + 4757/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
12.067, 11.485, 10.942, 10.433 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
12.002, 11.422, 10.881, 10.373 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
11.28; 10.99 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
11.31, 11.26 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Bioconcentration and Uptake and Elimination Rate Constants (K_1 and K_2):

k_1 = 170 L d^{-1} g^{-1} dry wt; k_2 = 0.123 d^{-1} in blue mussels (Gustafsson et al. 1999)
k_1 = 0.066 g org. C g^{-1} lipid h^{-1}; k_2 = 0.022 d^{-1} in Lake Höytiäinen sediment; k_1 = 0.99 g org. C g^{-1} lipid h^{-1}; k_2 = 0.026 d^{-1} in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)

Half-Lives in the Environment:

Air: first order degradation $t_{½}$ = 467 h (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first order degradation $t_{½}$ = 14400 h (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Biota: depuration $t_{½}$ = 5.6 d in blue mussels (Gustafsson et al. 1999);
biphasic depuration kinetics observed in oligochaete tissues with $t_{½}$ = 10.5–47.5 h in compartment A for sediment ingesting oligochaetes (Leppänen & Kukkonen 2004)

TABLE 10.1.5.23.1
Reported octanol-air partition coefficients of 2,2′,4,4′,5-pentabromodiphenyl ether (PBDE 99) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	11.847	15	12.067
25	11.321	25	11.485
35	10.887	35	10.942
45	10.258	45	10.433
25	11.31	QRSETP model 5	
		15	12.002
log K_{OA} = A + B/(T/K)		25	11.422
A	–4.64	35	10.881
B	4757	45	10.373
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 91.1			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

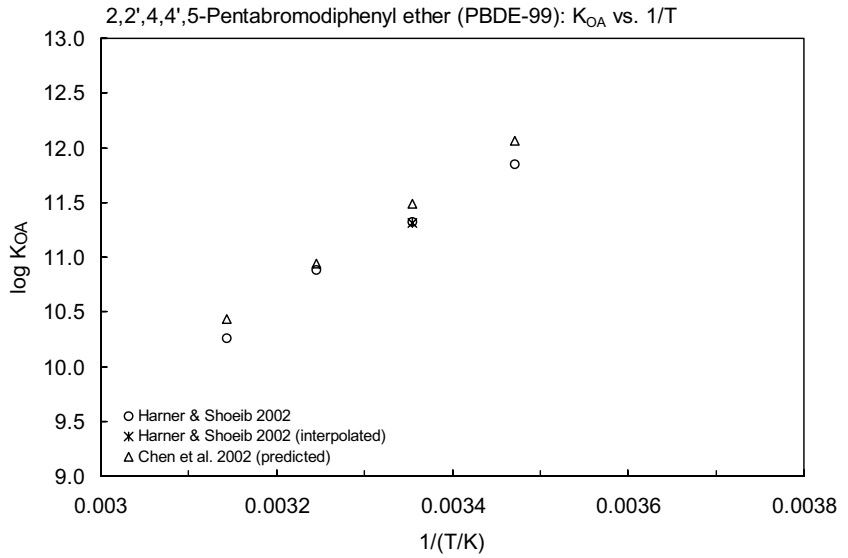
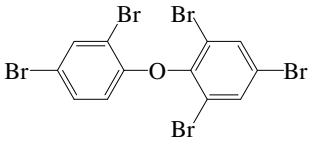


FIGURE 10.1.5.23.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2′,4,4′,5-pentabromodiphenyl ether (PBDE-99).

10.1.5.24 2,2′,4,4′,6-Pentabromodiphenyl ether (BDE-100)



Common Name: 2,2′,4,4′,6-Pentabromodiphenyl ether
Synonym: PBDE-100, 1,3,5-tribromo-2-(2,4-dibronphenoxy)-benzene
Chemical Name: 2,2′,4,4′,6-pentabromodiphenyl ether
CAS Registry No: 189084-64-8
Molecular Formula: $C_{12}H_5Br_5O$
Molecular Weight: 564.687
Melting Point (°C):
102 (Tittlemier et al. 2002)
110 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
312.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
102 (Tittlemier et al. 2002)
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:
0.179 (at mp 100.5°C, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at 25°C):
0.040 (generator column-GC/ECD, Tittlemier et al. 2002)
0.0499, 0.0541 (supercooled S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
7.33×10^{-5}–1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
2.86×10^{-5} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –5339/(T/K) + 13.37, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
3.99×10^{-5}, 3.68×10^{-5} (supercooled P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.069 (calculated-P_L/C_L, Tittlemier et al. 2002)
0.384 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
6.86 (estimated, Tittlemier et al. 2002)
6.51, 6.53 (selected measured value, final adjusted value, Wania & Dugani 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:
11.13* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –7.18 + 5459/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
11.721, 11.140, 10.596, 10.087 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
11.758, 11.179, 10.637, 10.130 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

11.20; 11.52 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
11.13, 11.02 (selected measured value, final adjusted value, Wania & Dugani 2003)

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:
Air: first order degradation $t_{½}$ = 357 h (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first order degradation $t_{½}$ = 14400 h (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Biota:

TABLE 10.1.5.24.1
Reported octanol-air partition coefficients of 2,2′,4,4′,6-pentabromodiphenyl ether (PBDE 100) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	11.755	15	11.721
25	11.185	25	11.14
35	10.509	35	10.596
45	9.993	45	10.087
25	11.13	QRSETP model 5	
		15	11.758
log K_{OA} = A + B/(T/K)		25	11.179
A	–7.18	35	10.637
B	5459	45	10.13
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 105.0			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

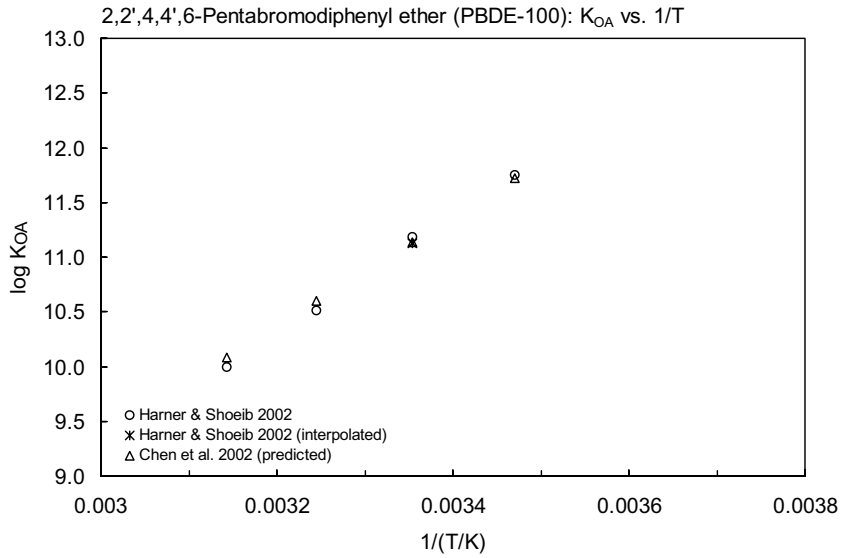
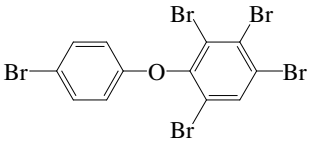


FIGURE 10.1.5.24.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2′,4,4′,6-pentabromodiphenyl ether (PBDE-100).

10.1.5.25 2,3,4,4′,6-Pentabromodiphenyl ether (BDE-115)



Common Name: 2,3,4,4′,6-Pentabromodiphenyl ether
Synonym: PBDE-115, BDE-115, 1,2,3,5-tetrabromo-4-(4-bromophenoxy)benzene
Chemical Name: 2,3,4,4′,6-pentabromodiphenyl ether
CAS Registry No: 446254-78-0
Molecular Formula: $C_{12}H_5Br_5O$
Molecular Weight: 564.687
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
312.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
101.8 (Wong et al. 2001)
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):
6.47×10^{-7} (calculated for penta-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
7.33×10^{-5}–1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.07 (estimated for penta-BDE, Alcock et al. 1999)
3.02×10^{-5}; 3.20×10^{-5} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -5219/(T/K) + 13.32$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
11.52; 11.20 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

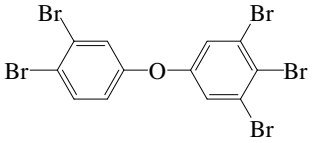
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.26 3,3′,4,4′,5-Pentabromodiphenyl ether (BDE-126)



Common Name: 3.3′,4,4′,5-Pentabromodiphenyl ether
Synonym: PBDE-126, BDE-126, 1,2,3-tribromo-5-(3,4-dibromophenoxy)-benzene
Chemical Name: 3,3′,4,4′,5-pentabromodiphenyl ether
CAS Registry No: 366791-32-4
Molecular Formula: $C_{12}H_5Br_5O$
Molecular Weight: 564.687
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
312.1 (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):
6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C):
7.33×10^{-5}–1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.07 (estimated for penta-PBDEs, Alcock et al. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

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:
11.97* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –8.41 + 6077/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
12.642, 12.001, 11.441, 10.611 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
12.544, 11.964, 11.423, 10.915 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

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 10.1.5.26.1
Reported octanol-air partition coefficients of 3,3′,4,4′,5-pentabromodiphenyl ether (PBDE 126) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	12.642	15	12.574
25	12.001	25	11.992
35	11.441	35	11.449
45	10.611	45	10.939
25	11.97	QRSETP model 5	
		15	12.544
log K_{OA} = A + B/(T/K)		25	11.964
A	–8.41	35	11.423
B	6077	45	10.915
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 116.0			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

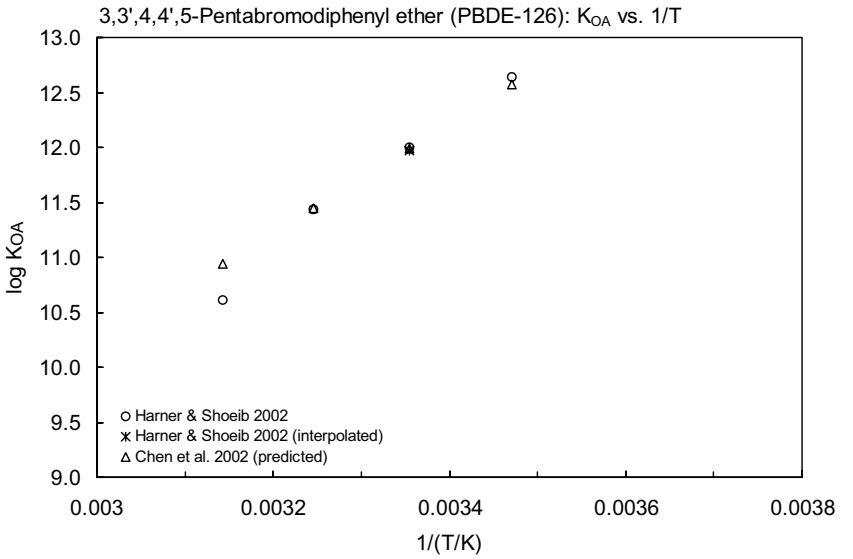
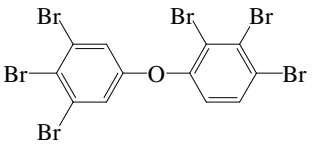


FIGURE 10.1.5.26.1 Logarithm of K_{OA} versus reciprocal temperature for 3,3′,4,4′,5-pentabromodiphenyl ether (PBDE-126).

10.1.5.27 2,3,3′,4,4′,5′-Hexabromodiphenyl ether (BDE-138)



Common Name: 2,3,3′,4,4′,5′-Hexabromodiphenyl ether
Synonym: PBDE-138, BDE-138, 1,2,3-tribromo-4-(2,4,5-tribromophenoxy)-benzene
Chemical Name: 2,3,3′,4,4′,5′-hexabromodiphenyl ether
CAS Registry No: 182677-30-1
Molecular Formula: $C_{12}H_4Br_6O$
Molecular Weight: 643.584
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
335.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
114.06 (Tittlemier & Tomy 2001)
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):
4.08×10^{-6} (calculated for hexaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
9.44×10^{-6}–4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.95–0.99 (estimated for hexa-BDE, Alcock et al. 1999)
1.51×10^{-6} (supercooled liquid P_L: GC-RT correlation, Tittlemier & Tomy 2001)
log (P_L/Pa) = –5957/(T/K) + 14.17, (GC-RT correlation, Tittlemier & Tomy 2001)
1.58×10^{-6} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –6191/(T/K) + 14.97, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)
7.91 (estimated, Tittlemier et al. 2002)

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

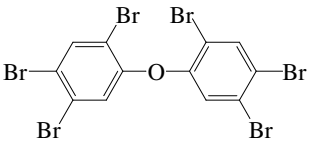
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.28. 2,2′,4,4′,5,5′-Hexabromodiphenyl ether (BDE-153)



Common Name: 2,2′,4,4′,5,5′-Hexabromodiphenyl ether
Synonym: PBDE-153, BDE-153, 1,1′-oxybis[2,4,5-tribromophenoxy)-benzene
Chemical Name: 2,2′,3,3′,5,5′-hexabromodiphenyl ether
CAS Registry No: 68631-49-2
Molecular Formula: $C_{12}H_4Br_6O$
Molecular Weight: 643.583
Melting Point (°C):
160–163 (Tittlemier et al. 2002)
161.5 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
335.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
107.6 (Wong et al. 2001)
110 (Tittlemier et al. 2002)
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:
0.045 (calculated at mp 161.5°C, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at 25°C):
4.08×10^{-6} (calculated for hexaBDE, Alcock et al. 1999)
8.70×10^{-7} (Solid S_S, generator column-GC/ECD, Tittlemier et al. 2002)
0.0195, 0.0167 (supercooled S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
9.44×10^{-6}–4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.95–0.99 (estimated for hexa-BDE, Alcock et al. 1999)
8.43×10^{-6}; 5.80×10^{-8} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
$\log (P_L/Pa) = -5620/(T/K) + 13.78$, (GC-RT correlation, Wong et al. 2001)
2.09×10^{-6} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
$\log (P_L/Pa) = -5763/(T/K) + 13.66$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
7.58×10^{-6}, 8.87×10^{-6} (supercooled P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.067 (calculated-P_L/C_L, Tittlemier et al. 2002)
0.342 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.86–7.93 (hexabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)
7.39 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)
7.62 (estimated, Tittlemier et al. 2002)
7.13, 7.08 (selected measured value, final adjusted value, Wania & Dugani 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:

11.82* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –5.39 + 5131/(T/K), temp range 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
12.708, 12.127, 11.583, 11.074 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
12.556, 11.977, 11.435, 10.928 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
12.15; 11.78 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
11.82, 11.89 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 19 L d^{-1} g^{-1} dry wt. in blue mussels (Gustafsson et al. 1999)
k_2 = 0.086 d^{-1} in blue mussels (Gustafsson et al. 1999)
k_2 = 0.051 d^{-1} with $t_{½}$ = 13.6 d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:
Air: first order degradation $t_{½}$ = 1110 h (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first order degradation $t_{½}$ = 14400 h (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Biota: depuration $t_{½}$ = 8.1 d in blue mussels (Gustafsson et al. 1999);
$t_{½}$ = 13.6 ± 9 d in carp (Stapleton et al. 2004a)
depuration $t_{½}$ = 13.6 d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.28.1
Reported octanol-air partition coefficients of 2,2′,4,4′,5,5′-hexabromodiphenyl ether (PBDE 153) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	12.318	15	12.708
25	11.86	25	12.127
35	11.569	35	11.583
45	10.534	45	11.074
25	11.82	QRSETP model 5	
		15	12.556
log K_{OA} = A + B/(T/K)		25	11.977
A	–5.39	35	11.435
B	5131	45	10.928
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 98.2			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

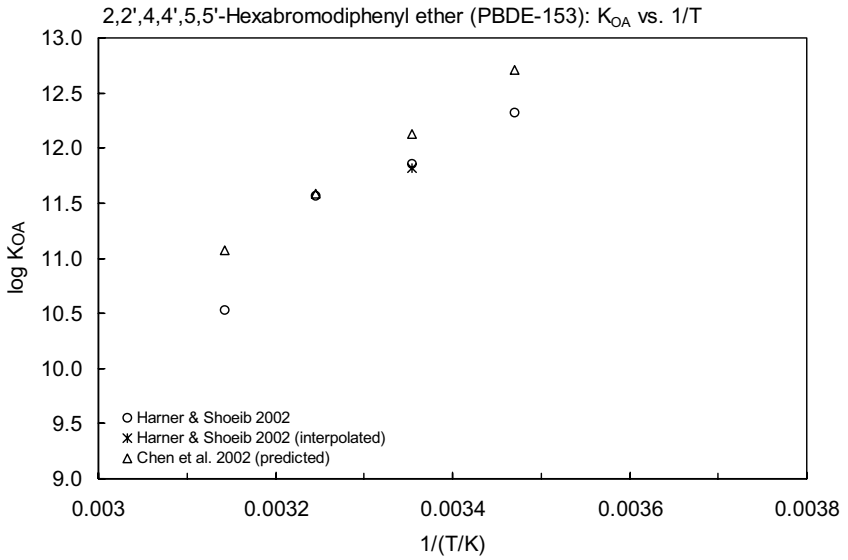
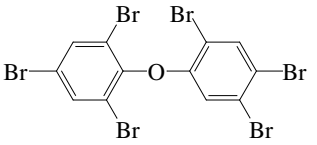


FIGURE 10.1.5.28.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2′,4,4′,5,5′-hexabromodiphenyl ether (PBDE-153).

10.1.5.29 2,2′,4,4′,5,6′-Hexabromodiphenyl ether (BDE-154)



Common Name: 2,2′,4,4′,5,6′-Hexabromodiphenyl ether
Synonym: PBDE-154, BDE-154, 1,3,5-tribromo-2-(2,4,5-tribromophenoxy)-benzene
Chemical Name: 2,2′,4,4′,5,6′-hexabromodiphenyl ether
CAS Registry No: 207122-15-4
Molecular Formula: $C_{12}H_4Br_6O$
Molecular Weight: 643.583
Melting Point (°C):
131–132.5 (Tittlemier et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
335.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
113 (Tittlemier et al. 2002)
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):
4.08×10^{-6} (calculated for hexa-PBDEs, Alcock et al. 1999)
8.70×10^{-7} (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at 25°C):
9.44×10^{-6}–4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.95–0.99 (estimated for hexa-PBDEs, Alcock et al. 1999)
3.80×10^{-6} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –5900/(T/K) + 14.38, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.24 (calculated-P_L/C_L, Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)
7.39 (estimated, Tittlemier et al. 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
11.92* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –4.62 + 4931/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
12.471, 11.890, 11.346, 10.837 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
12.361, 11.782, 11.240, 10.733 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

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

$k_2 = 2.0 \times 10^{-2}$ d^{-1} with $t_{½}$ = 35 d in juvenile carp (Stapleton et al. 2004a)

Half-Lives in the Environment:

Biota: depuration $t_{½}$ = 35 ± 18 d in juvenile carp (Stapleton et al. 2004a)

TABLE 10.1.5.29.1
Reported octanol-air partition coefficients of 2,2',4,4',5,6'-hexabromodiphenyl ether (PBDE 154) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	12.455	15	12.471
25	11.935	25	11.89
35	11.531	35	11.346
45	10.789	45	10.837
25	11.92	QRSETP model 5	
		15	12.361
log K_{OA} = A + B/(T/K)		25	11.782
A	–4.62	35	11.24
B	4931	45	10.733
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 94.4			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

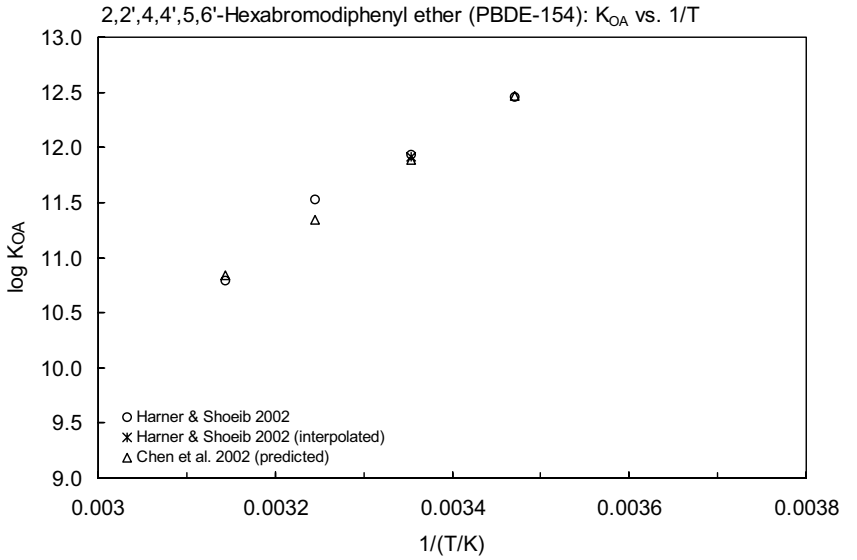
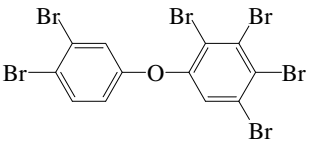


FIGURE 10.1.5.29.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2′,4,4′,5,6′-hexabromodiphenyl ether (PBDE-154).

10.1.5.30 2,3,3′,4,4′,5-Hexabromodiphenyl ether (BDE-156)



Common Name: 2,3,3′,4,4′,5-Hexabromodiphenyl ether
Synonym: PBDE-156, BDE-156, 1,2,3,4-tetrabromo-5-(3,4-dibromophenoxy)-benzene
Chemical Name: 2,3,3′,4,4′,5-hexabromodiphenyl ether
CAS Registry No: 405237-85-6
Molecular Formula: $C_{12}H_4Br_6O$
Molecular Weight: 643.583
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
335.4 (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):
4.08×10^{-6} (calculated for hexa-PBDEs, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C):
$9.44 \times 10^{-6} - 4.22 \times 10^{-6}$ (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.95–0.99 (estimated for hexa-PBDEs, Alcock et la. 1999)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

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:
11.97* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –5.80 + 5298/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
13.211, 12.630, 12.087, 11.577 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
13.150, 12.571, 12.029, 11.522 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

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 10.1.5.30.1
Reported octanol-air partition coefficients of 2,3,3′,4,4′,5′-hexabromodiphenyl ether (PBDE 156) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	-	15	13.211
25	11.976	25	12.63
35	-	35	12.087
45	10.858	45	11.577
25	11.97	QRSETP model 5	
		15	13.15
log K_{OA} = A + B/(T/K)		25	12.571
A	–5.80	35	12.029
B	5298	45	11.522
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 101.0			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

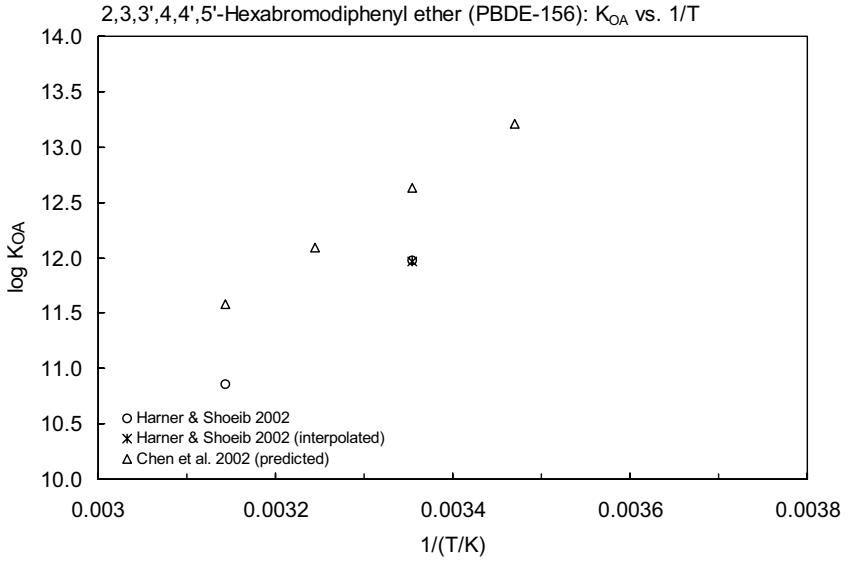
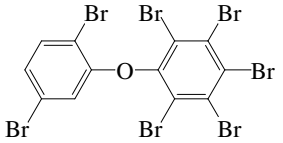


FIGURE 10.1.5.30.1 Logarithm of K_{OA} versus reciprocal temperature for 2,3,3′,4,4′,5-hexabromodiphenyl ether (PBDE-156).

10.1.5.31 2,2′,3,4,5,5′,6-Heptabromodiphenyl ether (BDE-183)



Common Name: 2,2′,3,4,5,5′,6-Heptabromodiphenyl ether
Synonym: PBDE-183, BDE-183, 1,2,3,5-tetrabromo-4-(2,4,5-trobromophenoxy)-benzene
Chemical Name: 2,2′,3,4,5,5′-heptabromodiphenyl ether
CAS Registry No: 207122-16-5
Molecular Formula: $C_{12}H_3Br_7O$
Molecular Weight: 722.479
Melting Point (°C):
171–173 (Tittlemier et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
358.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
118 (Tittlemier et al. 2002)
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:
0.035 (calculated at mp 172°C, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at 25°C):
1.50×10^{-6} (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
4.68×10^{-7} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
$\log (P_L/Pa) = -6185/(T/K) + 14.43$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0074 (calculated-P_L/C_L, Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (quoted, Wania & Dugani 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:
11.96* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
$\log K_{OA} = -3.71 + 4672/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
13.263, 12.681, 12.138, 11.628 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
13.206, 12.627, 12.085, 11.577 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

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:
Air: first-order degradation $t_{½}$ = 1540 h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first-order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first order degradation $t_{½}$ = 14400 h (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)
Biota:

TABLE 10.1.5.31.1
Reported octanol-air partition coefficients of 2,3,3′,4,4′,5′-hexabromodiphenyl ether (PBDE 183) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	-	15	13.263
25	11.964	25	12.681
35	11.477	35	12.138
45	10.978	45	11.628
25	11.96	QRSETP model 5	
		15	13.206
log K_{OA} = A + B/(T/K)		25	12.627
A	–3.71	35	12.085
B	4672	45	11.577
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 89.5			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

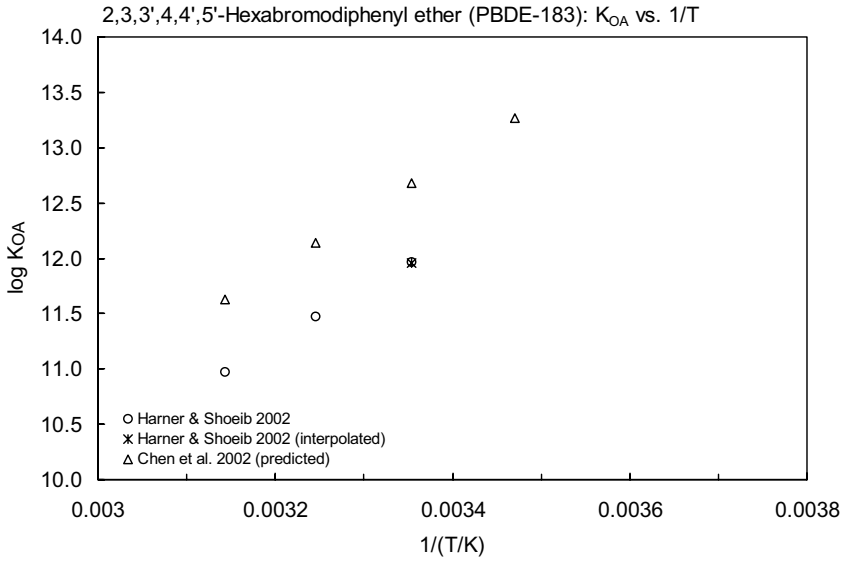
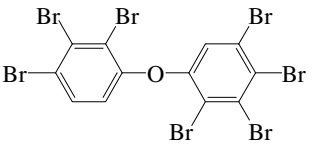


FIGURE 10.1.5.31.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2′,3,4,4′,5′,6-heptabromodiphenyl ether (PBDE-183).

10.1.5.32 2′,3,3′,4,4′,5,6-Heptabromodiphenyl ether (BDE-190)



Common Name: 2′,3,3′,4,4′,5,6-Heptabromodiphenyl ether
Synonym: PBDE-190, BDE-190, pentabromo-(3,4-dibromophenoxy)-benzene
Chemical Name: 2′,3,3′,4,4′,5,6-heptabromodiphenyl ether
CAS Registry No: 189084-68-2
Molecular Formula: $C_{12}H_3Br_7O$
Molecular Weight: 722.479
Melting Point (°C):
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
358.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
121.15 (Tittlemier & Tomy 2001)
115.8 (Wong et al. 2001)
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 at 25°C and reported temperature dependence equation):
2.34×10^{-7} (supercooled liquid P_L: GC-RT correlation, Tittlemier & Tomy 2001)
log (P_L/Pa) = –6327/(T/K) + 14.60, (GC-RT correlation, Tittlemier & Tomy 2001)
9.05×10^{-7}; 5.70×10^{-7} (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –6048/(T/K) + 14.24, (GC-RT correlation, Wong et al. 2001)
2.82×10^{-7} (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –6552/(T/K) + 15.44, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
8.36 (estimated, Tittlemier et al. 2002)

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

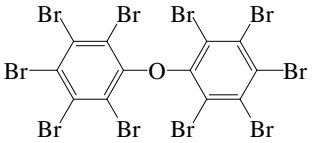
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

10.1.5.33 Decabromodiphenyl ether (BDE-209)



Common Name: Decabromodiphenyl ether
Synonym: PBDE-209, BDE-209, 1,1′-oxybis[2,3,4,5,6-pentabromo]-benzene, bis(pentabromophenyl)-ether, 102(E), 2,2′,3,3′,4,4′,5,5′,6,6′-decabromodiphenyl ether, Decabromobiphenyl oxide, decabromophenyl ether
Chemical Name: decabromodiphenyl ether
CAS Registry No: 1163-19-5
Molecular Formula:$C_{12}Br_{10}O$
Molecular Weight: 959.167
Melting Point (°C):
302.5 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
428.6 (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):
4.17×10^{-9} (solid S_S, quoted lit., Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C):
2.95×10^{-9} (supercooled liquid P_L, estimated, Wania & Dugani 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
9.97 (decabromodiphenyl ether, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
9.97 (quoted from Watanabe & Tatsukawa 1990, Pijnenburg et al. 1995)
9.97 (quoted, Wania & Dugani 2003)

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, $t_{½}$:
Volatilization:
Photolysis: half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{½} < 0.25$ h on silica gel, $t_{½}$ = 12 h on sand, $t_{½}$ = 40–60 h on sediment and $t_{½}$ = 150–200 h in soil; for outdoors under sunlight "discontinuous": $t_{½}$ = 37 h on sand and 80 h on sediment; for outdoor sunlight "continuous": $t_{½}$(calc) = 13 h on sand and $t_{½}$(calc) = 30 on sediment (Södertröm et al. 2004)
Photooxidation:
Hydrolysis:
Biodegradation: anaerobic degradation decreased by 30% within 238 d corresponding to a pseudo-first-order $k = 1 \times 10^{-3}$ d^{-1} by sewage sludge collected from a mesophilic digester (Gerecke et al. 2005)

Biotransformation:

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

$k_2 = 1.4 \times 10^{-2}$ d^{-1} with $t_{½}$ = 50 d in juvenile carp (Stapleton et al. 2004)

Half-Lives in the Environment:

Air: first order degradation $t_{½}$ = 7620 h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{½}$ = 14400 h (estimated by EPIWIN, Wania & Dugani 2003); photolysis half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{½}$ = 40–60 h on sediment; for outdoors under sunlight "discontinuous": $t_{½}$ = 80 h on sediment; for outdoor sunlight "continuous": $t_{½}$(calc) = 30 on sediment (Södertröm et al. 2004)

Soil: first order degradation $t_{½}$ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003); photolysis half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{½}$ = 12 h on sand, and 150–200 h in soil; for outdoors under sunlight "discontinuous": 37 h on sand; for outdoor sunlight "continuous": $t_{½}$(calc) = 13 h on sand (Södertröm et al. 2004)

Biota: depuration $t_{½}$ = 50 ± 17 d in juvenile carp (Stapleton et al. 2004)

TABLE 10.2.1
Summary of physical properties of ethers and halogenated ethers

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/m³ at 20°C	Molar volume, V_M cm³/mol	
								MW/ρ at 20°C	Le Bas
Aliphatic ethers:									
Dimethyl ether (Methyl ether)	115-10-6	$(CH_3)_2O$	46.068	–141.5	–24.8	1	0.6689	68.87	60.9
Diethyl ether (Ethyl ether)	60-29-7	$(C_2H_5)_2O$	74.121	–116.2	34.5	1	0.71361	103.87	106.1
Methyl *t*-butyl ether (MTBE)	1634-04-4	$CH_3OC(CH_3)_3$	88.148	–108.6	55	1	0.7404	119.05	127.5
Di-*n*-propyl ether	111-43-3	$(C_3H_7)_2O$	102.174	–114.8	90.08	1	0.7466	136.85	151.6
Di-isopropyl ether	108-20-3	$((CH_3)_2CH)_2O$	102.174	–85.4	68.4	1	0.73	139.96	151.6
Butyl ethyl ether	628-81-9	$(C_4H_9)O(C_2H_5)$	102.174	–124	92.3	1	0.7495	136.32	150.5
Di-*n*-butyl ether	142-96-1	$(C_4H_9)_2O$	130.228	–95.2	140.28	1	0.7684	169.48	196
1,2-Propylene oxide	75-56-9	C_3H_6O	58.079	–111.9	35	1			69.7
Furan	110-00-9	C_4H_4O	68.074	–85.61	31.5	1	0.9378	72.59	73.5
2-Methylfuran	534-22-5	C_5H_6O	82.101	–91.3	64.7	1	0.9132	89.90	95.7
Tetrahydrofuran	109-99-9	C_4H_8O	72.106	–108.44	65	1	0.8892	81.09	88.3
Tetrahydropyran	142-68-7	$C_5H_{10}O$	86.132	–49.1	88	1	0.8814	97.72	107
1,4-Dioxane	123-91-1	$C_4H_8O_2$	88.106	11.85	101.5	1	1.0336	85.24	92
Halogenated ethers:									
Epichlorohydrin	106-89-8	C_3H_5ClO	92.524	–26	118	1	1.18066	78.37	90.6
Chloromethyl methyl ether	107-30-2	$ClCH_2$-O-CH_3	80.513	–103.5	59.5	1	1.0703	75.22	81.8
Bis(2-chloromethyl)ether	542-88-1	$C_2H_4Cl_2O$	114.958	–41.5	106	1			102.7
Bis(2-chloroethyl)ether	111-44-4	$(ClC_2H_4)_2O$	143.012	–51.9	178.5	1	1.2192	117.30	147.9
Bis(2-chloroisopropyl)ether	108-60-1	$(ClC_3H_6)_2O$	171.064	–97	187	1	1.11	154.11	193.4
2-Chloroethyl vinyl ether	110-75-8	ClC_2H_4-O-C_2H_3	106.551	–70	108	1	1.0475	101.72	119.6
Bis(2-chloroethoxy)methane	111-91-1	$(ClC_2H_4)_2O_2CH_2$	173.037		215	1			180.0
Aromatic ethers:									
Anisole (Methoxybenzene)	100-66-3	$(C_6H_5)O(CH_3)$	108.138	–37.13	153.7	1	0.994	108.79	127.3
2-Chloroanisole	766-51-8	C_7H_7ClO	142.583	–26.8	198.5	1	1.1911	119.71	148.2
3-Chloroanisole	2845-89-8	C_7H_7ClO	142.583		193.5				148.2
4-Chloroanisole	227881	C_7H_7ClO	142.583	< –18	197.5	1	1.201	118.72	148.2
2,3-Dichloroanisole	1984-59-4	$C_7H_6Cl_2O$	177.028	32		0.854			169.1
2,6-Dichloroanisole	1984-65-2	$C_7H_6Cl_2O$	177.028	10		1			169.1

(Continued)

TABLE 10.2.1 *(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/m³ at 20°C	Molar volume, V_M cm³/mol	
								MW/ρ at 20°C	Le Bas
2,3,4-Trichloroanisole	54135-80-7	$C_7H_5Cl_3O$	211.473	70		0.362			190.0
2,4,6-Trichloroanisole	87-40-1	$C_7H_5Cl_3O$	211.473	61.5	241	0.438			190.0
2,3,4,5-Tetrachloroanisole	938-86-3	$C_7H_4Cl_4O$	245.918	88		0.241			210.9
2,3,5,6-Tetrachloroanisole	6936-40-9	$C_7H_4Cl_4O$	245.918	84		0.264			210.9
Veratrole (1,2-Dimethoxybenzene)	91-16-7	$C_8H_{10}O_2$	138.164	22.5	206	1			158.6
4,5-Dichloroveratrole	2772-46-5	$C_8H_8Cl_2O_2$	207.054	83		0.270			200.4
3,4,5-Trichloroveratrole	16766-29-3	$C_8H_7Cl_3O_2$	241.499	66		0.396			221.3
Tetrachloroveratrole	944-61-6	$C_8H_6Cl_4O_2$	275.944	90		0.230			242.2
Phenetole (Ethoxybenzene)	103-73-1	$(C_6H_5)O(C_2H_5)$	122.164	–29.43	169.81	1	0.9651	126.58	150.3
Benzyl ethyl ether	539-30-0	$C_6H_5CH_2OC_2H_5$	136.190		186	1	0.949	143.51	172.5
Styrene oxide	96-09-3	C_8H_8O	120.149	–35.6	194.1	1	1.0500	114.43	136.1
Diphenyl ether	101-84-8	$C_{12}H_{10}O$	170.206	26.87	258	0.959	1.0748	158.36	195.6

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 10.2.2
Summary of selected physical-chemical properties of ethers and halogenated ethers at 25°C

	Selected properties						
	Vapor pressure		Solubility				Henry's law constant H/(Pa·m³/mol) calculated P/C
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}	
Aliphatic ethers:							
Dimethyl ether (Methyl ether)	600000	600000	353000	7662	7662	0.1	13.22*
Diethyl ether (Ethyl ether)	71600	71600	60500	816.2	816.2	0.89	87.72
Methyl *t*-butyl ether (MTBE)	33500	33500	42000	476.5	476.5	0.94	70.31
Di-*n*-propyl ether	8334	8334	3306	32.35	32.35	2.03	257.6
Di-isopropyl ether	20000	20000	7900	77.31	77.31	1.52	258.7
Butylethyl ether	8200	8200	6500	63.61	63.61	2.03	128.9
Di-*n*-butyl ether	850	850	230	1.766	1.776	3.21	481.3
1,2-Propylene oxide	71000	71000	476000	8196	8196	0.03	8.663
Furan	80000	80000	10000	146.9	146.9	1.34	544.6
Tetrahydrofuran	21600	21600	miscible				
Tetrahydropyran	9536	9536	85700	995.0	995.0	0.82	9.584
1,4-Dioxane	5000	5000	miscible			0.27	
Halogenated ethers:							
Epichlorohydrin	2400	2400	65800	771.2	711.2	0.30	3.37
Chloromethyl methyl ether	24900	24900	decompose				
Bis(chloromethyl)ether	4000	4000	22000	191.4	191.4	0.38	20.90
Bis(2-chloroethyl)ether	206	206	10200	71.32	71.32	1.12	2.888
Bis(2-chloroisopropyl)ether	104	104	1700	9.938	9.938	2.58	10.46
2-Chloroethyl vinyl ether	3566	3566	15000	140.8	140.8	1.28	25.33
Bis(2-chloroethoxy)methane	21.6	21.6	81000	468.1	468.1	1.26	0.0461
Aromatic ethers:							
Anisole (Methoxybenzene)	472	472	1600	14.80	14.80	2.11	31.90
2-Chloroanisole			490	3.436	3.436	2.50	
3-Chloroanisole			235	1.648		2.60	
4-Chloroanisole			237	1.662	1.662	2.70	
2,3-Dichloroanisole			86.9	0.4909	0.5748	3.24	
2,6-Dichloroanisole			13.12	0.0741	0.0741	3.14	

(*Continued*)

TABLE 10.2.2 *(Continued)*

	Selected properties						
	Vapor pressure		Solubility				Henry's law constant H/(Pa·m³/mol) calculated P/C
Compound	**P^S/Pa**	**P_L/Pa**	**S/(g/m³)**	**C^S/(mol/m³)**	**C_L/(mol/m³)**	**log K_{OW}**	
2,3,4-Trichloroanisole			10.8	0.0511	0.1411	4.03	
2,4,6-Trichloroanisole			13.2	0.0624	0.1425	4.02	
2,3,4,5-Tetrachloroanisole			1.35	0.0055	0.0228	4.50	
2,3,5,6-Tetrachloroanisole			1.82	0.0074	0.0280	4.40	
Veratrole (1,2-Dimethoxybenzene)			6690	48.42	48.42	2.18	
4,5-Dichloroveratrole			72	0.2477	1.2879	3.11	
3,4,5-Trichloroveratrole			10.3	0.0426	0.1077	4.01	
Tetrachloroveratrole			1.59	0.0058	0.0250	4.86	
Phenetole (Ethoxybenzene)	204	204	569	4.658	4.658	2.68	43.80
Benzyl ethyl ether	100	100				2.64	
Styrene oxide	40	40	2800	23.30	23.0	1.61	1.716
Diphenyl ether	2.93	3.05	18.7	0.1099	0.1146	4.21	26.67

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H (Pa·m³/mol) = 101325 Pa/C^S mol/m³.

TABLE 10.2.3
Suggested half-life classes of ethers and halogenated ethers in various environmental compartments at 25°C

Compound	Air class	Water* class	Soil class	Sediment class
Aliphatic ethers:				
Dimethyl ether (Methyl ether)	2	5	5	6
Diethyl ether (Ethyl ether)	2	5	5	6
Methyl *t*-butyl ether (MTBE)	2	5	5	6
Di-*n*-propyl ether	2	5	5	6
1,2-Propylene oxide	2	4	5	6
Furan	2	4	5	6
Tetrahydrofuran	2	4	5	6
1,4-Dioxane	2	4	5	6
Halogenated ethers:				
Chloromethyl methyl ether	2	5	5	6
Bis(chloromethyl)ether	2	5	5	6
Bis(2-chloroethyl)ether	2	5	5	6
Bis(2-chloroisopropyl)ether	2	5	5	6
2-Chloroethyl vinyl ether	2	5	5	6
Bis(2-chloroethoxy)methane	2	5	5	6
Aromatic ethers:				
Anisole (Methoxybenzene)	2	5	5	6
Styrene oxide	2	4	5	6
Diphenyl ether	2	5	5	6

* Certain ethers will have much shorter half-lives because of hydrolysis with singlet oxygen, and biodegradation; this half-life class is conservatively assigned, see Chapter 1 for a discussion.

where,

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 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

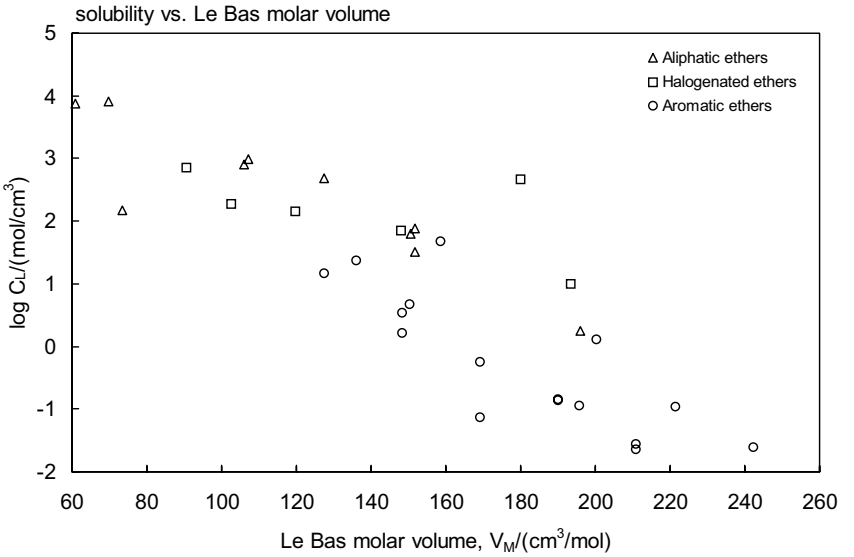


FIGURE 10.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for ethers.

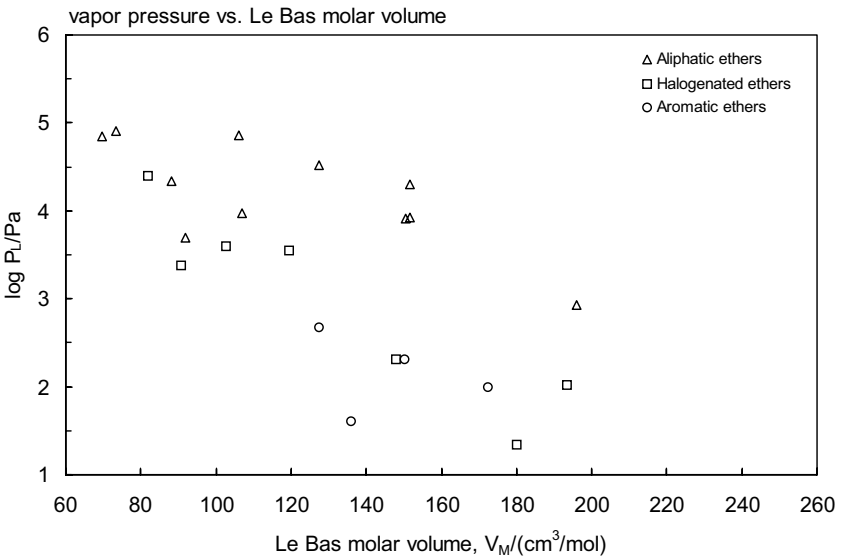


FIGURE 10.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for ethers.

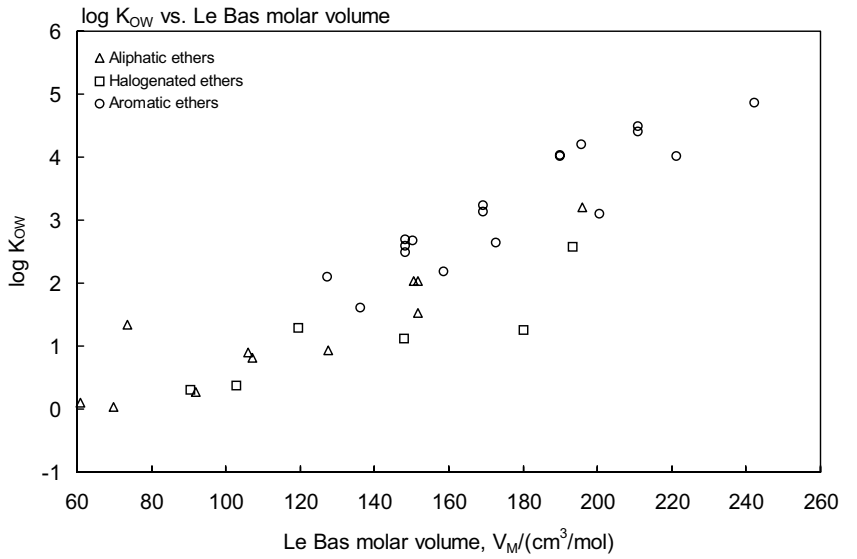


FIGURE 10.2.3 Octanol-water partition coefficient versus Le Bas molar volume for ethers.

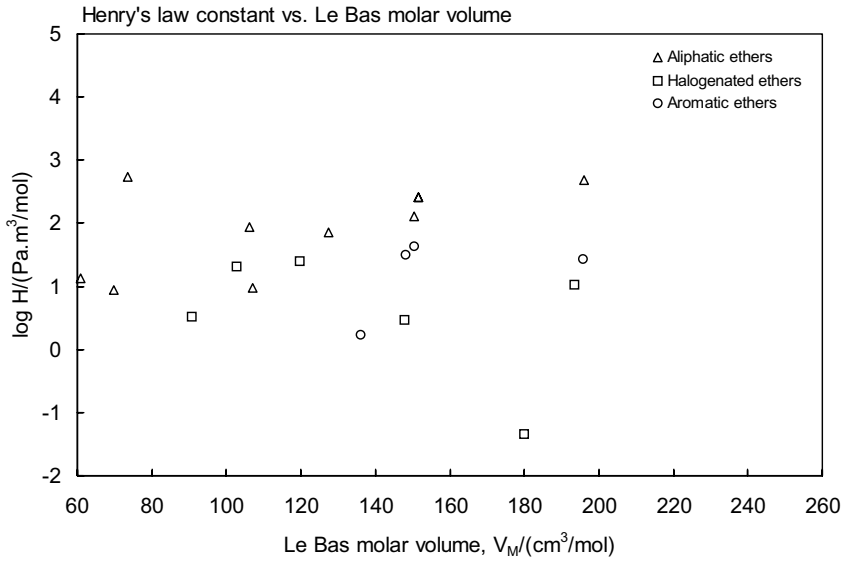


FIGURE 10.2.4 Henry's law constant versus Le Bas molar volume for ethers.

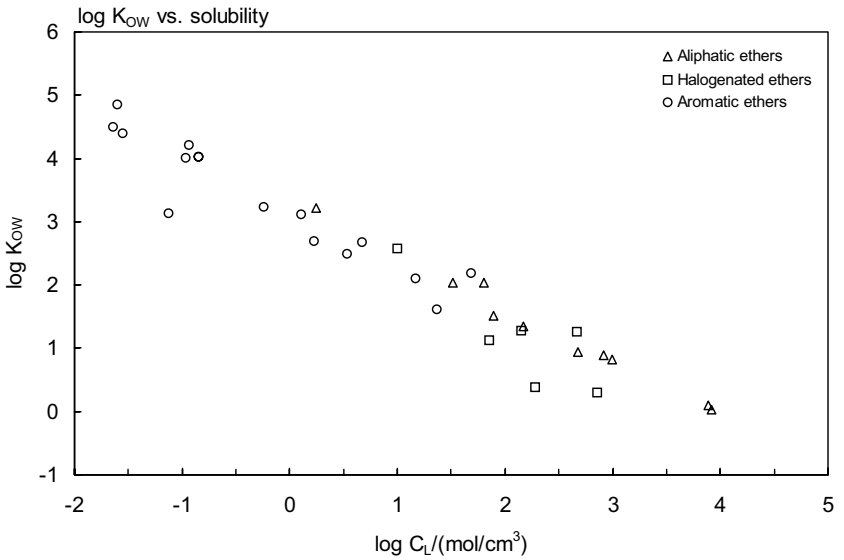


FIGURE 10.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for ethers.

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