
9 Chlorinated Dibenzofurans

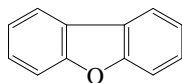
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9.1 LIST OF CHEMICALS AND DATA COMPILATIONS

9.1.1 DIBENZOFURAN AND CHLORINATED DIBENZOFURANS

9.1.1.1 Dibenzofuran



Common Name: Dibenzofuran

Synonym: diphenylene oxide

Chemical Name: dibenzofuran

CAS Registry No: 132-64-9

Molecular Formula: $C_{12}H_8O$, $C_6H_4OC_6H_4$

Molecular Weight: 168.191

Melting Point ($^{\circ}C$):

86.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

287 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0886 ($99^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

154.4 ($99^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

147.8 (Ruelle & Kesselring 1997)

176.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

65.4 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

85.63 (Rordorf 1989)

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

19.6 (Rordorf 1987, 1989; quoted, Ruelle & Kesselring 1997)

18.6 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

54 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.249 (mp at $86.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3.11 (Lu et al. 1978)

10.03 (shake flask-HPLC/UV, Banerjee et al. 1980)

6.56 (selected average, Pearlman et al. 1984)

4.22* (generator column-GC, measured range $4-39.8^{\circ}C$, Doucette & Andren 1988a)

$S/(mol/L) = 8.32 \times 10^{-6} \exp(0.041 \cdot t/^{\circ}C)$; temp range $4-40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a); or

$\log x = -1558/(T/K) - 1.135$; temp range $4-40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

3.36 (calculated-TSA, Dickhut et al. 1994)

4.30 (computed-expert system SPARC, Kollig 1995)

$4.75^* \pm 0.22$ (generator column-HPLC/UV, Shiu et al. 1997)

4.69 ± 0.18 (shake flask-GC, Shiu et al. 1997)

2.43 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle Kesselring 1997)

17.21; 62.49 (supercooled liquid S_L , quoted lit. average; calculated-SOFA-Solubility parameters for Fate Analysis model, Govers & Krop 1998)

$\ln x = -1.6385 - 3842.2/(T/K)$; temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

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

- 0.276* (gas saturation, extrapolated-Antoine eq. from exptl. data, measured temp range, 30–70°C, Hansen & Eckert 1986)
- 0.506* (26°C, gas saturation exptl. data, measured range 49–74°C, Sato et al. 1986)
- 0.466 (gas saturation-GC, extrapolated-Antoine eq. derived from exptl. data, temp range 49–74°C, Sato et al. 1986)
- 0.35* (gas saturation-GC, measured range 25–125°C Rordorf 1986, 1989)
- 2.026 (extrapolated liquid value P_L , Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 5.8968 - 1851.27/(-82.64 + T/K)$; temp range 403–559 K (Antoine eq., Stephenson & Malanowski 1987)
- 0.40 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
- $\log(P/\text{mmHg}) = 17.6646 - 3.1989 \times 10^3/(T/K) - 3.3346 \cdot \log(T/K) + 6.0686 \times 10^{-10} \cdot (T/K) + 4.4676 \times 10^{-7} \cdot (T/K)^2$; temp range 356–838 K (vapor pressure eq., Yaws et al. 1994)
- 0.360 (computed-expert system SPARC, Kollig 1995)
- 0.708; 0.123 (supercooled liquid P_L , quoted exptl. or exptl. average; calculated-SOFA model (Solubility parameters of Fate Analysis model), Govers & Krop 1998)
- $\log(P/\text{Pa}) = 13.17192 - 4083/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.429 (gas saturation-HPLC/fluorescence, de Seze et al. 2000)
- 0.398* (25.2°C, Knudsen effusion method, measured range 20.2–45°C Li et al. 2002)
- $\ln(P/\text{Pa}) = 33.54 - 10313/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2002 2004)
- $\ln(P/\text{Pa}) = (32.203 \pm 0.576) - (9880.4 \pm 176)/(T/K)$; temp range 295–318 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C):

- 14.16 (calculated-P/C with selected values)
- 14.20 (computed-expert system SPARC, Kollig 1995)
- 21.38, 13.80 (calculated-P/C, Govers & Krop 1998)

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

- 4.12 (HPLC-RT correlation, Veith et al. 1979a)
- 4.12 (Hansch & Leo 1979)
- 4.17 (shake flask-HPLC/UV, Banerjee et al. 1980)
- 3.91, 4.12, 4.18; 3.96, 4.10, 4.17 (HPLC-RT, linear regressions; quadratic regressions, Sarna et al. 1984)
- 3.92 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
- 4.31 (generator column-GC/ECD, both phases, Doucette & Andren 1987)
- 3.86 (HPLC-RT correlation, Doucette & Andren 1988b)
- 4.21, 3.81 (shake flask-HPLC, TLC-RT correlation, De Voogt et al. 1990)
- 4.12 (recommended, Sangster 1993)
- 4.12 (recommended, Hansch et al. 1995)
- 4.27 (generator column-HPLC/UV, Shiu et al. 1997)
- 4.273* (shake flask-HPLC/UC, measured S_O and S_W , Shiu et al. 1997)
- 4.09 ± 0.19 , 4.12 ± 0.63 ; 4.12 (HPLC- k' correlation: ODS-65 column, Diol-35 column; quoted lit average value, Helweg et al. 1997)

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

Bioconcentration Factor, $\log BCF$:

- 3.13 (fathead minnow, 28 d exposure, Veith et al. 1979b)
- 3.13, 2.80 (quoted exptl., calculated- K_{OW} , Mackay 1982)
- 3.13, 3.13 (quoted exptl., calculated-MCI χ , Sabljic 1987)

- 3.13 (calculated- K_{OW} , Isnard & Lambert 1989)
 3.68; 4.08 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.80 (computed- K_{OW} , Kollig 1995)
 4.15 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)
 3.45 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 3.84 (soil-pore-water partition coeff. for Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)

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

Volatilization:

Photolysis:

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

$k_{OH} = 3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ corresponding to an atmospheric lifetime of about 8 h (Atkinson 1987a)

$k_{OH} = 3.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1987b)

$t_{1/2} = 1.9\text{--}19 \text{ h}$ based on estimated rate constant with OH radicals in air (Howard 1991)

$k_{OH} = 31 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ the tropospheric lifetime was calculated to be 0.5 d (Atkinson 1991)

$k_{OH} = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and with calculated tropospheric lifetime of 3.7 d; $k_{NO_3} < 7 \times 10^{-30} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $>7 \text{ yr}$ and $k_{O_3} < 8 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with O_3 with calculated tropospheric lifetime $>250 \text{ d}$ at room temp. (Kwok et al. 1994)

$k_{OH}(\text{exptl}) = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ corresponding to a tropospheric lifetime of 3.7 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegradation $t_{1/2} \sim 168\text{--}672 \text{ h}$ and anaerobic $t_{1/2} = 672\text{--}2688 \text{ h}$, based on aerobic acclimated and unacclimated groundwater die-away test data (Lee et al. 1984; quoted, Ward et al. 1986; Howard et al. 1991); nonautoclaved groundwater samples at hazardous waste site with a concentration of approximate 0.09 mg/L are degraded by microbes at rates about 30% per week while the levels of the controls decreased only about half that rate (Lee et al. 1984).

Biotransformation:

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

Half-Lives in the Environment:

Air: the calculated atmospheric lifetime range from $\sim 60\text{--}120 \text{ h}$ (Atkinson 1987a);

$t_{1/2} = 1.9\text{--}19 \text{ h}$, based on estimated rate constants for reaction with OH radicals (Howard et al. 1991);

the tropospheric lifetime was calculated 0.5 d for the gas-phase reaction for OH radicals using a 12-h average daytime OH radical concn of 1.5×10^6 (Atkinson 1991);

calculated room temp. tropospheric lifetimes of 3.7 d for reaction with OH radical, $>7 \text{ yr}$ with NO_3 radical, and $>250 \text{ d}$ for reaction with O_3 (Kwok et al. 1994);

room temp. tropospheric lifetime was calculated to be 3.7 d for reaction with OH radical (Kwok et al. 1995).

Surface water: $t_{1/2} = 168\text{--}672 \text{ h}$, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).

Groundwater: $t_{1/2} = 205\text{--}835 \text{ h}$, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672 \text{ h}$, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).

Biota:

TABLE 9.1.1.1
Reported aqueous solubilities and octanol-water partition coefficients of dibenzofuran at various temperatures

Aqueous solubility				Octanol-water partition coefficient	
Shiu et al. 1997		Doucette & Andren 1988a		Shiu et al. 1997	
generator column-HPLC/UV		generator column-GC/ECD		generator column-HPLC/UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	log K _{OW}
5	1.914	3.9	1.652	5	4.405
15	3.004	25	4.222	15	4.346
25	4.75	39.8	6.963	25	4.273
35	7.56			35	4.190
45	11.8	ΔH _{sol} /(kJ mol ⁻¹) = 29.8 for 4–32°C		45	4.116
shake flask-HPLC/UV				ΔH/(kJ mol ⁻¹) = −12.4	
25	4.69				
ΔH _{sol} /(kJ mol ⁻¹) = 33.3 5–45°C					

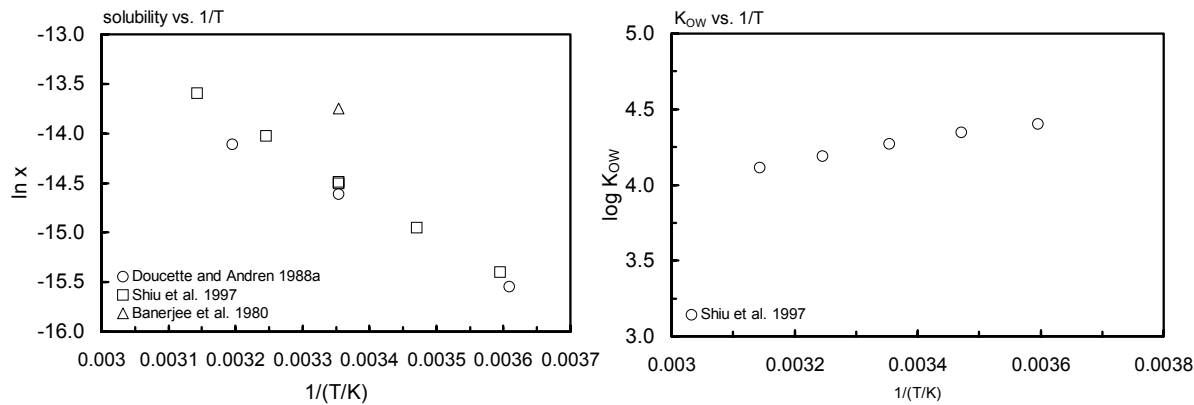


FIGURE 9.1.1.1 Logarithm of mole fraction solubility and K_{OW} versus reciprocal temperature for dibenzofuran.

TABLE 9.1.1.2

Reported vapor pressures of dibenzofuran at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Hanson & Eckert 1986		Sato et al. 1986		Rordorf 1989		Li et al. 2002	
gas saturation-IR		gas saturation-electrobalance		gas saturation-GC		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30	0.4874	25.85	0.506	25	0.35	20.2	0.284
35	0.7818	35.85	1.48	50	5.10	25.2	0.398
40	1.280	40.75	2.35	75	50.0	30	0.665
45	2.128	45.85	3.71	100	360	35	1.22
50	3.200	52.45	6.69	125	2100	40	1.94
55	4.679	55.65	8.8			45	3.04
60	7.246	59.75	12.5	$\Delta H_v/(\text{kJ mol}^{-1}) = 65.4$		eq. 1	P/Pa
65	12.78	60.35	13.5	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 85.630$			
70	19.71	64.45	18.3	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 19.6$			
		65.05	19.9	$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 54$			
$\log (P/\text{mPa}) = B - A/(T/K)$		66.15	21.5			B	9880.4
A	16.30	68.75	26.1				
B	4132	69.35	27.1				
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 79.1$		72.75	35.4				
		eq. 3	P/Pa				
		A	22.1098				
		B	4707.68				
		C	-92.332				

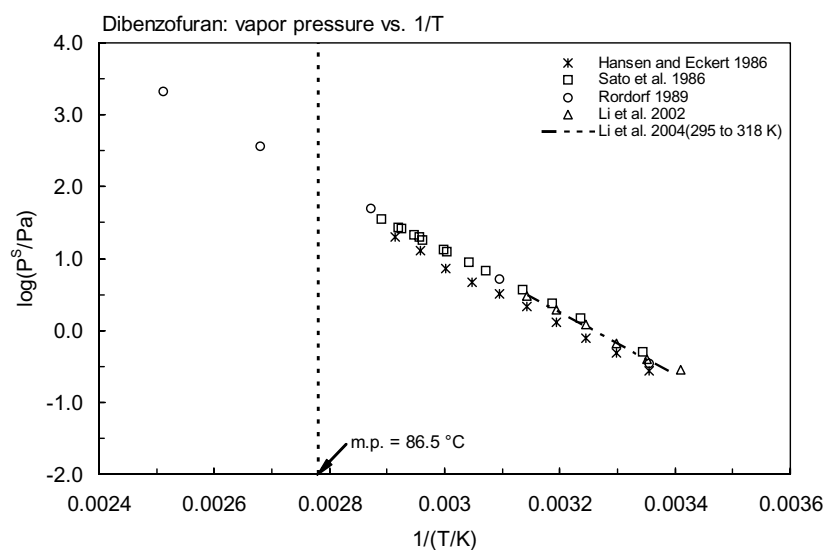
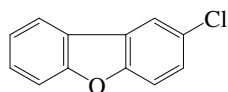


FIGURE 9.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for dibenzofuran.

9.1.1.2 2-Chlorodibenzofuran



Common Name: 2-Chlorodibenzofuran

Synonym: 2-MCDF

Chemical Name: 2-Chlorodibenzofuran

CAS Registry No: 51230-49-0

Molecular Formula: $C_{12}H_7ClO$, $C_6H_4OC_6H_3Cl$

Molecular Weight: 202.637

Melting Point ($^{\circ}C$):

101.5–102.5 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

338.2 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

197.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

75.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

95.28 (Rordorf 1989)

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

19.4 (Rordorf 1987, 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

52 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

11.66 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

4.23, 11.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

9.6×10^{-3} , 0.190, 2.40, 22.0, 150 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

0.537 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 40.57 - 5556/(T/K) - 9.999 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

0.174; 0.537 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

9.12 (calculated-SOFA model, Govers & Krop 1998)

10.23; 9.12 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

5.15; 4.37 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.51 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

4.77; 4.51 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

4.38 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

3.96; 4.38 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH} = (16-22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a mono-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 0.7–1.0 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991) $k_{OH}(\text{calc}) = (5.0-5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 2.9 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a mono-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 0.7–1.0 d (Atkinson 1991);

calculated tropospheric lifetime was 2.9 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

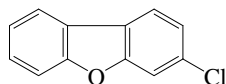
Ground water:

Sediment:

Soil:

Biota:

9.1.1.3 3-Chlorodibenzofuran



Common Name: 3-Chlorodibenzofuran

Synonym: 3-MCDF

Chemical Name: 3-Chlorodibenzofuran

CAS Registry No: 25074-67-3

Molecular Formula: $C_{12}H_7ClO$, $C_6H_4OC_6H_3Cl$

Molecular Weight: 202.637

Melting Point ($^{\circ}C$):

101–102 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

338.2 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

197.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

75.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

95.313 (Rordorf 1989)

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

19.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

52 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

12.21 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

6.34; 12.21 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.970, 0.190, 2.40, 22.0, 150 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

0.490 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 40.57 - 5553/(T/K) - 9.999 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

0.174; 0.490 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

7.76 (calculated-SOFA model, Govers & Krop 1998)

10.23; 7.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.35 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

5.15; 4.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.53 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

4.77; 4.53 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.34 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
3.96; 4.34 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

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

$k_{OH} = (16-22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a mono-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 0.7–1.0 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (5.0-5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 2.9 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a mono-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 0.7–1.0 d (Atkinson 1991);
calculated tropospheric lifetime of 2.9 d for with OH radical (Kwok et al. 1995).

Surface water:

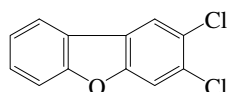
Ground water:

Sediment:

Soil:

Biota:

9.1.1.4 2,3-Dichlorodibenzofuran



Common Name: 2,3-Dichlorodibenzofuran

Synonym: 2,3-DCBF

Chemical Name: 2,3-dichlorodibenzofuran

CAS Registry No: 64126-86-9

Molecular Formula: $C_{12}H_6Cl_2O$

Molecular Weight: 237.082

Melting Point ($^{\circ}C$):

125.5–127 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

375 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

218.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

105.04 (Rordorf 1989)

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

25.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

63 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.50 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.716; 1.50 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.50×10^{-4} , 1.7×10^{-2} , 0.29, 3.20, 27.0 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

0.0282 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 39.20 - 5757/(T/K) - 9.466 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

0.1096; 0.0282 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

4.365 (calculated-SOFA model, Govers & Krop 1998)

4.79; 4.365 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.11 (calculated-SOFA model, Govers & Krop 1998)

5.43; 5.11 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{oa}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.82 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

5.04; 4.82 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

5.39 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

5.15; 5.39 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

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

$k_{OH} = (6.6-16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.6-3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 0.7–1.0 d (Atkinson 1991);

room temp. tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical (Kwok et al. 1995).

Surface water:

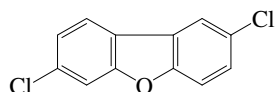
Ground water:

Sediment:

Soil:

Biota:

9.1.1.5 2,7-Dichlorodibenzofuran



Common Name: 2,7-Dichlorodibenzofuran

Synonym: 2,7-DCBF

Chemical Name: 2,7-dichlorodibenzofuran

CAS Registry No: 73992-98-6

Molecular Formula: $C_{12}H_8Cl_2O$

Molecular Weight: 237.082

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

218.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

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

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.32 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.785; 2.32 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0501 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 39.23 - 5755/(T/K) - 9.466 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

0.0123; 0.0501 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

5.01 (calculated-SOFA model, Govers & Krop 1998)

4.90; 5.01 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.02 (calculated-SOFA model, Govers & Krop 1998)

5.41; 5.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.79 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

5.03; 4.79 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{oc}$:

5.27 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

5.10; 5.27 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: photolysis $k = 0.23 \text{ min}^{-1}$ with $t_{1/2} = 3.0 \text{ min}$ in pure water and $k = 0.011 \text{ min}^{-1}$ with $t_{1/2} = 63 \text{ min}$ in 60 % acetonitrile/water solution in Corex centrifuge bottles at 300 nm photochemical reactor (Kim & O'Keefe 2000)

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

$k_{\text{OH}} = (6.6\text{--}16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.6\text{--}3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 0.7–1.0 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical at room temp. (Kwok et al. 1995).

Surface water:

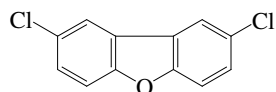
Ground water:

Sediment:

Soil:

Biota:

9.1.1.6 2,8-Dichlorodibenzofuran



Common Name: 2,8-Dichlorodibenzofuran

Synonym: 2,8-DCDF

Chemical Name: 2,8-dichlorodibenzofuran

CAS Registry No: 5409-83-6

Molecular Formula: $C_{12}H_6Cl_2O$

Molecular Weight: 237.082

Melting Point ($^{\circ}C$):

184–185 (Kuroki et al. 1984)

Boiling Point ($^{\circ}C$):

375 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

218.5 (calculated-Le Bas method at normal boiling point)

173.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

74.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

101.423 (Rordorf 1989)

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

25.1 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

18.6 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

55 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0145* (generator column-GC, measured range 4.5 – $39.5^{\circ}C$, Doucette & Andren 1988a)

$S/(mol/L) = 1.24 \times 10^{-6} \exp(0.082 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range 4 – $40^{\circ}C$, Doucette & Andren 1988a); or

$\log x = -2344/(T/K) - 1.093$; temp range 4 – $40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

0.024 (calculated-TSA, Dickhut et al. 1994)

0.0431 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

2.11 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\ln x = -2.515 - 5398.4/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.75; 2.11 (supercooled liquid S_L , GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

9.6×10^{-4} (estimated, van den Berg & Olie 1985)

3.9×10^{-4} * (calculated-bp and ΔH_{fus} , Rordorf 1987, 1989)

0.0145; 0.0417 (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log (P/Pa) = 14.30669 - 5281.67/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. from literature data, Shiu & Ma 2000)

0.0115; 0.0417 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

1.06×10^{-3} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

0.0412 (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56 J/mol K$, Mader & Pankow 2003)

$\log (P_L/mmHg) = 39.21 - 5756/(T/K) - 9.466 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/\text{Pa}) = 32.943 - 12162/(T/\text{K})$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (36.010 \pm 0.393) - (13262 \pm 144)/(T/\text{K})$; temp range 348–383 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

6.31; 4.57 (quoted lit.; calculated-SOFA model, Govers & Krop 1998)
 4.79; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

5.56, 5.97, 6.16; 5.65, 5.95, 6.15 (HPLC-RT correlation, linear regressions; quadratic regressions, Sarna et al. 1984)
 5.30 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
 5.44 (generator column-GC/ECD, Doucette & Andren 1987)
 5.12 (HPLC-RT correlation, Doucette & Andren 1988b)
 5.65 (recommended, Sangster 1993)
 5.65 (recommended, Hansch et al. 1995)
 5.42 (GC-RI correlation; Wang & Wong 2003)

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

Bioconcentration Factor, $\log \text{BCF}$:

5.04 (guppy, Loonen et al. 1994a)
 5.04; 4.81 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 5.04; 4.81 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

5.30 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 5.13; 5.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: when 5 mg/L in methanol was irradiated by sunlight simulator more than 95% disappears within 48 h while a similar experiment with highly purified methanol solution reveals only very slow photolysis within the same period of irradiation and results were same with 10 mg/L in methanol solution (Crosby & Moilanen 1973; quoted, Choudhary & Hutzinger 1982);

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

$k_{\text{OH}} = (6.6\text{--}16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.6\text{--}3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 1.0–2.3 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radicals (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: mean biological $t_{1/2} \sim 11$ d in rainbow trout (Niimi 1986).

TABLE 9.1.6.1

Reported aqueous solubilities and vapor pressures of 2,8-dichlorodibenzofuran at various temperatures

Aqueous solubility		Vapor pressure	
Doucette & Andren 1988a		Rordorf 1989	
generator column-GC/ECD		vapor pressure correlation	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
4.5	0.00384	25	3.9×10^{-4}
25	0.0145	50	9.1×10^{-3}
39.5	0.0339	75	0.14
		100	1.40
		125	11.0
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 74.2$	
4–32 $^{\circ}\text{C}$		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 101.423$	
$S/(\text{mol/L}) = a \cdot \exp[b \cdot (t/^{\circ}\text{C})]$		$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 25.1$	
a		$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 55$	
b			
	1.24×10^{-8}		
	0.062		

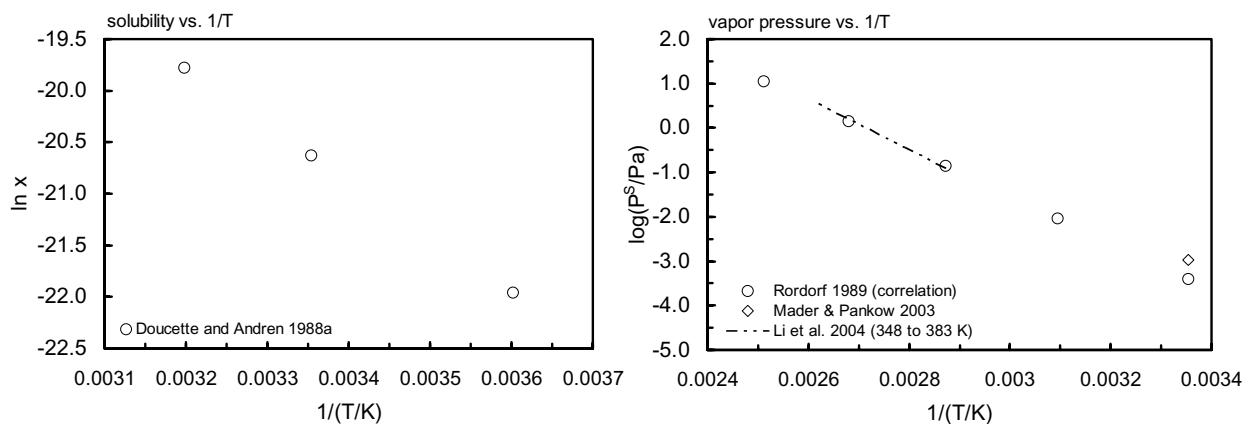
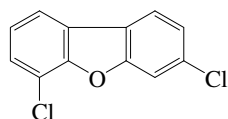


FIGURE 9.1.6.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,8-dichlorodibenzofuran.

9.1.1.7 3,6-Dichlorodibenzofuran



Common Name: 3,6-Dichlorodibenzofuran

Synonym: 3,6-DCDF

Chemical Name: 3,6-dichlorodibenzofuran

CAS Registry No: 94570-83-9

Molecular Formula: $C_{12}H_6Cl_2O$

Molecular Weight: 237.082

Melting Point ($^{\circ}C$):

188 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

357 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

218.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.7 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

110.87 (Rordorf 1989)

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

38.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

83 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0252 (mp at $188^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.76 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.684; 1.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.0×10^{-4} , 6.3×10^{-3} , 0.12, 1.60, 15 (25, 50, 75, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1985a,b, 1987, 1989)

0.0355 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

0.0123; 0.0355 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log(P_L/mmHg) = 39.18 - 5755/(T/K) - 9.466 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

4.57 (calculated-SOFA model, Govers & Krop 1998)

4.68; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.08 (calculated-SOFA model, Govers & Krop 1998)

5.44; 5.08 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.81 (lipid wt. basis, calculated-SOFA model, Govers & Krop 1998)

5.05; 4.81 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

5.35 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

5.18; 5.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

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

$k_{OH} = (6.6-16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.6-3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 1.0–2.3 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical (Kwok et al. 1995).

Surface water:

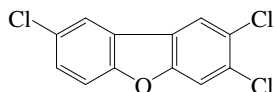
Ground water:

Sediment:

Soil:

Biota: mean biological $t_{1/2} = 24$ d in rainbow trout (Niimi & Oliver 1986)

9.1.1.8 2,3,8-Trichlorodibenzofuran



Common Name: 2,3,8-Trichlorodibenzofuran

Synonym: 2,3,8-TCDF

Chemical Name: 2,3,8-trichlorodibenzofuran

CAS Registry No: 57117-32-5

Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$

Molecular Weight: 271.527

Melting Point ($^{\circ}C$):

189–191 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

408.4 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

239.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

111.823 (Rordorf 1989)

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

30.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

67 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.291 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.113, 0.291 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.0×10^{-5} , 9.9×10^{-4} , 2.0×10^{-2} , 0.26, 2.50 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

4.27×10^{-3} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

9.12×10^{-4} , 4.27×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

2.48×10^{-4} (solid P_S , gas saturation-GC/MS, Mader & Pankow 2003)

0.0108 (supercooled liquid P_L , calculated from P_S assuming $\Delta S_{fus} = 56\ J/mol\ K$, Mader & Pankow 2003)

$\log(P_L/mmHg) = 37.66 - 5911/(T/K) - 8.932 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.24 (calculated-SOFA model, Govers & Krop 1998)

2.57; 3.24 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.76 (calculated-SOFA model, Govers & Krop 1998)

5.75; 5.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.94 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.20; 4.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.30 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.26; 6.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

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

$k_{OH} = (3.4-12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tri-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.3–4.5 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.5-2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 5.5–9.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991);

calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

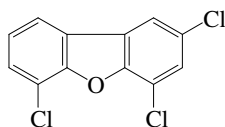
Ground water:

Sediment:

Soil:

Biota:

9.1.1.9 2,4,6-Trichlorodibenzofuran



Common Name: 2,4,6-Trichlorodibenzofuran

Synonym: 2,4,6-PCDF

Chemical Name: 2,4,6-trichlorodibenzofuran

CAS Registry No: 58802-14-6

Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$

Molecular Weight: 271.527

Melting Point ($^{\circ}C$):

116–117 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

408.4 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

239.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

116.061 (Rordorf 1989)

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

30.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

79 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.461 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.175; 0.461 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

5.33×10^{-4} (estimated, Van den Berg & Olie 1985)

8.2×10^{-5} , 3.1×10^{-3} , 6.8×10^{-2} , 1.0, 10.0 ($25, 50, 75, 100, 125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

4.27×10^{-3} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

1.32×10^{-3} , 4.27×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

9.22×10^{-4} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

7.50×10^{-3} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56\ J/mol\ K$, Mader & Pankow 2003)

$\log(P_L/mmHg) = 37.77 - 5908/(T/K) - 8.932 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/Pa) = 37.264 - 13912/(T/K)$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln(P/Pa) = (35.837 \pm 0.729) - (13090 \pm 259)/(T/K)$; temp range 338–373 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.40 (calculated-SOFA model, Govers & Krop 1998)

2.82; 2.40 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.64 (calculated-SOFA model, Govers & Krop 1998)

5.69; 5.64 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.99 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.18; 4.99 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.12 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 6.09; 6.12 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

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

$k_{OH}(\text{calc}) = (3.4 - 4.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (3.4 - 12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 1.3–4.5 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a tri-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.5 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 4.0–5.5 d for a tri-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991); calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical for a tri-chlorinated dibenzofuran (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

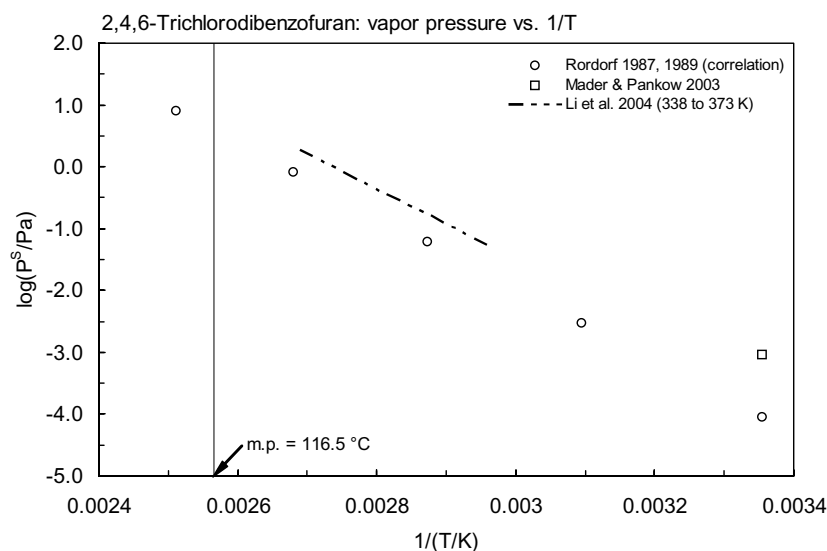
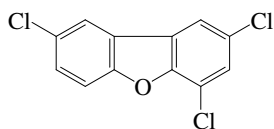


FIGURE 9.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trichlorodibenzofuran.

9.1.1.10 2,4,8-Trichlorodibenzofuran



Common Name: 2,4,8-Trichlorodibenzofuran

Synonym: 2,4,8-TCDF

Chemical Name: 2,4,8-trichlorodibenzofuran

CAS Registry No: 54589-71-8

Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$

Molecular Weight: 271.527

Melting Point ($^{\circ}C$):

155–156 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

392.5 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

239.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.7 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

112.3 (Rordorf 1989)

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

32.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

76 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0542 (mp at $154^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.494 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.157; 0.494 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

9.1×10^{-5} * (gas saturation-GC, Rordorf 1989)

5.75×10^{-3} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 37.78 - 5809/(T/K) - 8.932 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.38×10^{-3} , 5.75×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.09 (calculated-SOFA model, Govers & Krop 1998)

2.88; 3.09 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.64 (calculated-SOFA model, Govers & Krop 1998)

5.69; 5.64 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.94 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.18; 4.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Sorption Partition Coefficient, log K_{OC} :

6.14 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

6.06; 6.14 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

Volatilization:

Photolysis:

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

$k_{OH} = (3.4-12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tri-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.3–4.5 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.5-2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 5.5–9.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991);

calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 9.1.10.1
Reported vapor pressures of 2,4,8-tetrachlorodibenzofuran at various temperatures

Rordorf 1987, 1989	
gas saturation-GC	
$t/^{\circ}\text{C}$	P/Pa
25	9.1×10^{-5}
50	3.0×10^{-3}
75	6.1×10^{-2}
100	0.82
125	8.0
$\Delta H_v/(\text{kJ mol}^{-1}) = 78.7$	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 112.3$	
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 32.6$	
$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 76$	

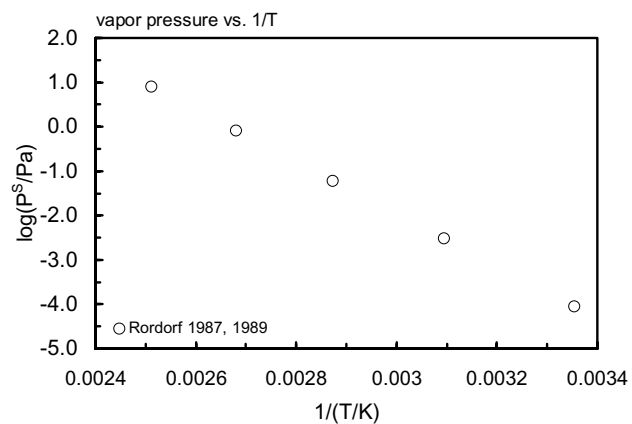
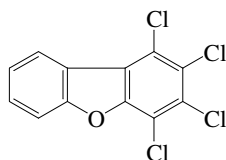


FIGURE 9.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,8-trichlorodibenzofuran.

9.1.1.11 1,2,3,4-Tetrachlorodibenzofuran



Common Name: 1,2,3,4-Tetrachlorodibenzofuran

Synonym: 1,2,3,4-TCDF

Chemical Name: 1,2,3,4-tetrachlorodibenzofuran

CAS Registry No: 24478-72-6

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

168.5–169 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.4 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

122.826 (Rordorf 1989)

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

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

83 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0717 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0306; 0.0717 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.1×10^{-6} , 1.9×10^{-4} , 5.1×10^{-3} , 8.7×10^{-2} , 1.0 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

6.76×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 36.02 - 6019/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.17×10^{-4} , 6.76×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.75 (calculated-SOFA model, Govers & Krop 1998)

1.74; 2.75 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.17 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)

6.34 (calculated-SOFA model, Govers & Krop 1998)

6.07; 6.34 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.92 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.22; 4.92 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.12 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.18; 7.12 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctance solution, and solid phase photolysis half-life, $t_{1/2} = 95$ h with PCDF dispersed as solid films (Buser 1988)

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

$k_{OH} = (1.4\text{--}8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8\text{--}1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 154, 134 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 > 1.8, > 1.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}, 220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_5 CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCF_s for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

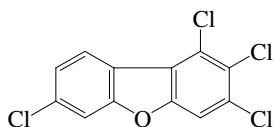
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: half-lives in gold fish: $t_{1/2} < 0.4$ d for PBO treated and $t_{1/2} > 0.5$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.12 1,2,3,7-Tetrachlorodibenzofuran



Common Name: 1,2,3,7-Tetrachlorodibenzofuran

Synonym: 1,2,3,7-TCDF

Chemical Name: 1,2,3,7-tetrachlorodibenzofuran

CAS Registry No: 83704-22-7

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

167.5–168 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.4 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

122.879 (Rordorf 1989)

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

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

83 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0805 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0306; 0.0805 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.2×10^{-6} , 1.9×10^{-4} , 5.2×10^{-3} , 8.9×10^{-2} , 1.1 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.08×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

1.41×10^{-4} , 7.08×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log(P_L/mmHg) = 36.07 - 6015/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

2.57 (calculated-SOFA model, Govers & Krop 1998)

1.78; 2.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.31 (calculated-SOFA model, Govers & Krop 1998)

6.04; 6.31 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.41 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)

4.93 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.23; 4.93 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

7.07 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

7.10; 7.07 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase photolysis $t_{1/2} = 95$ h with PCDF dispersed as solid films (Buser 1988)

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

$k_{OH}(\text{calc}) = (4.9 - 6.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.4 - 8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 1.9\text{--}11$ d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8 - 1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 7.7\text{--}18$ d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 142 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.007 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}$, $220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCF_s for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

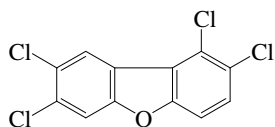
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} = 96$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.13 1,2,7,8-Tetrachlorodibenzofuran



Common Name: 1,2,7,8-Tetrachlorodibenzofuran

Synonym:

Chemical Name: 1,2,7,8-tetrachlorodibenzofuran

CAS Registry No: 58802-20-3

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

210–211 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

81.5 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

120.604 (Rordorf 1989)

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

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

76 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0496 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0273; 0.0496 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.67×10^{-4} (estimated, Van den Berg et al. 1985)

1.30×10^{-4} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

2.4×10^{-6} , 1.0×10^{-4} , 2.610^{-3} , 4.2×10^{-2} , 0.49 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

3.55×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 35.97 - 6020/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.047×10^{-4} , 3.35×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.09 (calculated-SOFA model, Govers & Krop 1998)

1.70; 2.09 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.23 (shake flask-slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989)

6.41 (calculated-SOFA model, Govers & Krop 1998)

5.964 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)

6.10; 6.41 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.97 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.22; 4.97 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.20 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.24; 7.20 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase photolysis half-life, $t_{1/2} = 35$ h with PCDF dispersed as solid films (Buser 1988);

$k = 0.014 \text{ min}^{-1}$ with $t_{1/2} = 50$ min in pure water and $k = 0.0041 \text{ min}^{-1}$ with $t_{1/2} = 170$ min in 60 % acetonitrile/water solution in Corex centrifuge bottles at 300 nm photochemical reactor; $k = 0.08 \text{ h}^{-1}$ with $t_{1/2} = 8.3$ h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000)

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

$k_{OH} = (1.4\text{--}8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8\text{--}1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 162, 130 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.14, >1.0 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}$, $220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

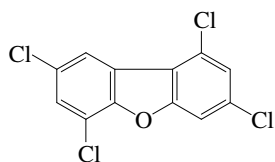
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} = 4.9$ d for PBO treated goldfish, and $t_{1/2} < 0.7$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.14 1,3,6,8-Tetrachlorodibenzofuran



Common Name: 1,3,6,8-Tetrachlorodibenzofuran

Synonym:

Chemical Name: 1,3,6,8-tetrachlorodibenzofuran

CAS Registry No: 71998-72-6

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

177–178 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

122.36 (Rordorf 1989)

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

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

81 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.212 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0625; 0.212 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.6×10^{-6} , 1.6×10^{-4} , 4.3×10^{-3} , 7.4×10^{-2} , 0.88 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

1.17×10^{-3} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 36.34 - 6020/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

2.95×10^{-4} , 1.17×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.62 (calculated-SOFA model, Govers & Krop 1998)

2.04; 1.62 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.37 (shake flask/slow stirring-GC/MS, fly-ash extract, Sijm et al. 1989)

6.06 (calculated-SOFA model, Govers & Krop 1998)

5.92; 6.06 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, log BCF or log K_B :

- 5.0 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.23; 5.0 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

- 6.71 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.76; 6.71 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

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

$k_{OH} = (1.4-8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8-1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radicals (Kwok et al. 1995).

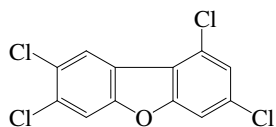
Surface water:

Ground water:

Sediment: degradation $t_{1/2} = 20-200 \text{ yr}$ in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota:

9.1.1.15 1,3,7,8-Tetrachlorodibenzofuran

Common Name: 1,3,7,8-Tetrachlorodibenzofuran

Synonym: 1,3,7,8-TCDF

Chemical Name: 1,3,7,9-tetrachlorodibenzofuran

CAS Registry No: 57117-35-8

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 306

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

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

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.116 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0463; 0.116 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and the reported temperature dependence equations):

6.03×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

2.00×10^{-4} , 6.03×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

3.51×10^{-5} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

$\log(P_L/mmHg) = 36.20 - 6020/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.55 (calculated-SOFA model, Govers & Krop 1998)

1.91; 1.55 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.39 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)

6.20 (calculated-SOFA model, Govers & Krop 1998)

5.98; 6.20 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.83 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)

5.01 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.23; 5.01 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

6.90 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

6.95; 6.90 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (4.9 - 6.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991) $k_{OH} = (1.4 - 8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 1.9\text{--}11 \text{ d}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991) $k_{OH}(\text{calc}) = (0.8 - 1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 7.7\text{--}18 \text{ d}$ for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2): $k_1 = 164, 293 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, > 1.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993) $k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}, 220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a tetra-CDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

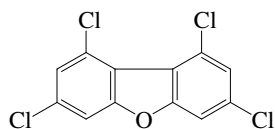
Surface water:

Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} > 7 \text{ d}$ for PBO treated goldfish and $t_{1/2} < 0.5 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.16 1,3,7,9-Tetrachlorodibenzofuran

Common Name: 1,3,7,9-Tetrachlorodibenzofuran

Synonym: 1,3,7,9-TCDF

Chemical Name: 1,3,7,9-tetrachlorodibenzofuran

CAS Registry No: 64560-17-4

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

206.5–207.5 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.3 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

121.988 (Rordorf 1989)

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

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

80 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.104 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0422; 0.104 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.5×10^{-6} , 1.1×10^{-4} , 2.7×10^{-3} , 4.5×10^{-2} , 0.51 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

4.37×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

1.78×10^{-4} , 4.36×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log(P_L/mmHg) = 36.15 - 6018/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.26 (calculated-SOFA model, Govers & Krop 1998)

1.86; 1.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.39 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)

6.22 (calculated-SOFA model, Govers & Krop 1998)

6.00; 6.22 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.83 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)

5.06 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.23; 5.06 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

6.91 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

7.00; 6.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

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

$k_{OH}(\text{calc}) = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.4\text{--}8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8\text{--}1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 164, 293 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, > 1.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}, 220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCF_s for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

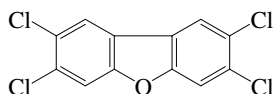
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} > 7 \text{ d}$ for PBO treated gold fish and $t_{1/2} < 0.5 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.17 2,3,7,8-Tetrachlorodibenzofuran



Common Name: 2,3,7,8-Tetrachlorodibenzofuran

Synonym: 2,3,7,8-TCDF

Chemical Name: 2,3,7,8-Tetrachlorodibenzofuran

CAS Registry No: 51207-31-9

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

227 (Lide 2003)

Boiling Point ($^{\circ}C$):

438.3 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

199.4 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

80.3 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

119.699 (Rordorf 1989)

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

36.6 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

73.2 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.0104 (calculated-assuming $\Delta S_{fus} = 56 J/mol K$ and $mp = 227^{\circ}C$)

0.00256 (calculated- ΔS_{fus} and mp , Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.19×10^{-4} ($22.7^{\circ}C$, generator column-HPLC/LSC, Friesen et al. 1990)

3.51×10^{-3} (calculated-QSAR, Fiedler & Schramm 1990)

4.20×10^{-4} ; 5.32×10^{-4} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.0413; 0.0413 (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.655 - 1915/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

0.0243; 0.0413 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.0×10^{-6} (quoted, Van den Berg & Olie 1985)

2.0×10^{-6} , 8.5×10^{-5} , 2.1×10^{-3} , 3.3×10^{-2} , 0.38 (25 , 50 , 75 , 100 , $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

1.23×10^{-4} (GC-RT correlation, supercooled liquid P_L , Eitzer & Hites 1988, 1991; quoted, Della Site 1997)

1.13×10^{-4} (GC-RT correlation, supercooled liquid P_L , Eitzer & Hites 1989; quoted, Della Site 1997)

2.00×10^{-4} (supercooled liquid P_L , Falconer & Bidleman 1994; quoted, Kaupp & McLachlan 1999)

1.23×10^{-6} , 1.13×10^{-6} (calculated from reported P_L , solid vapor pressures, Della Site 1997)

7.50×10^{-4} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)

1.62×10^{-4} ; 3.72×10^{-4} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

7.39×10^{-4} ; 1.89×10^{-6} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.48 - 5425/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.66 - 3513/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

- 1.678×10^{-5} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)
 1.718×10^{-3} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56$ J/mol K, Mader & Pankow 2003)
 $\log (P_L/\text{mmHg}) = 35.91 - 6019/(T/K) - 8.399 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 8.91×10^{-5} , 3.72×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 1.50 (calculated for tetrachloro-PCDFs, Eitzer & Hites 1989)
 1.70 (gas stripping-GC, 21°C , Friesen et al. 1993)
 1.17; 2.69 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 8.01 - 1598/(T/K)$ (Passivirta et al. 1999)
 1.66; 2.69 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 5.82 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 6.53 (shake flask/slow stirring-GC/MS, from mixture of fly ash extract, Sijm et al. 1989)
 6.19 (correlated, Ma et al. 1990)
 7.10 (calculated-QSAR, Fiedler & Schramm 1990)
 7.70 (calculated, Broman et al. 1991)
 5.83 (HPLC-RT correlation, Jackson et al. 1993)
 6.53 (recommended, Hansch et al. 1995)
 6.46 (calculated-SOFA model, Govers & Krop 1998)
 6.46, 6.58 (quoted, calculated-solubility $\log S_L$ and regression from lit. $\log K_{ow}$, Passivirta et al. 1999)
 6.225 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 6.13; 6.46 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

- 9.42 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
 10.02; 9.44 (generator column-GC/ECD; calculated, Harner et al. 2000)
 10.90 (7°C , GC retention time correlation, Harner et al. 2000)
 $\log K_{OA} = -4.92 + 4450/(T/K)$; temp range $10\text{--}50^\circ\text{C}$ (Harner et al. 2000)

Bioconcentration Factor, $\log \text{BCF}$:

- 4.82 (guppy, Opperhuizen et al. 1986)
 3.78, 3.39 (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988)
 3.64, 3.41 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
 3.82 (guppy, quoted, Opperhuizen & Sijm 1990)
 4.19; 4.12 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.19; 4.33; 5.02 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.93 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.23, 6.53 (fish with 5% lipid: wet weight basis, lipid weight basis, Geyer et al. 2000)
 6.54, 5.75 (fish muscle $\log \text{BCF}_L$ calculated from water, sediment, Wu et al. 2001)
 5.22; 4.93 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{oc}$:

- 5.20 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 7.50 (calculated, Broman et al. 1991)
 6.62 (calculated- K_{ow} , Kollig 1993)
 5.18; 5.34 (sediment in lake mesocosm, Muir et al. 1992)
 7.08; 7.29 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.32; 7.29 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase $t_{1/2} = 120$ h with PCDF dispersed as solid films (Buser 1988);

photolytic $t_{1/2} = 9.8$ h in extract of fly-ash and in tetradecane solution for native congener and $t_{1/2} = 3.0$ h for ^{13}C -labelled congener (Tysklind & Rappe 1991).

Hydrolysis:

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

$k_{\text{OH}}(\text{calc}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1987b)

$k_{\text{O}_3} = 1.32 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$ oxidative degradation rate constant for water dissolved PCDF by ozone under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987);

$k_{\text{OH}}(\text{calc}) = (2.4 - 3.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (1.4 - 8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 1.9\text{--}11$ d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (0.8 - 1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 7.7\text{--}18$ d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

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

$k_1 = 400 \text{ d}^{-1}$; $k_2 = 0.062 \text{ d}^{-1}$ (guppy, exposed to fly-ash extract, Opperhuizen et al. 1986)

$k_1 = 1228, 6853 \text{ d}^{-1}$; $k_2 = 0.28, 2.60 \text{ d}^{-1}$ (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988)

$k_1 = 56, 453 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, 0.22 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}, 220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_3CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0058 \text{ d}^{-1}$ with a biological $t_{1/2} = 58$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 603 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.292 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994a)

$k_2 = 0.0263 \text{ d}^{-1}$ with $t_{1/2} = 26$ d (newly contaminated oysters, Gardinali et al. 2004)

$k_2 = 0.0194 \text{ d}^{-1}$ with $t_{1/2} = 36$ d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be 7.7–18 d for the gas-phase reaction with OH radical (Kwok et al. 1995);

$t_{1/2} = 320$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 90$ min in isooctane solution in summer sunlight (Palauscek & Scholz 1987);

suggested $t_{1/2} = 6400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{1/2} = 61$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (Suzuki et al. 2000)

$t_{1/2} = 550\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr in soil (Suzuki et al. 2000)

$t_{1/2} = 550\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: Elimination $t_{1/2} = 2$ d from rat (Birnbaum et al. 1980; quoted, Birnbaum 1985);

$t_{1/2} = 8$ d from monkey (Birnbaum et al. 1981; quoted, Birnbaum 1985);

$t_{1/2} = 2\text{--}4$ d from mouse (Decad et al. 1981b; quoted, Birnbaum 1985);

$t_{1/2} = 40$ d from guinea pig (Decad et al. 1981a; Ioannou et al. 1983; quoted, Birnbaum 1985);

elimination half-lives: in guinea pigs, 20 d; rats, < 2 d; monkeys, 8 d; and mice, 2–4 d (quoted,

Van den Berg & Olie 1985);

$t_{1/2} < 336$ d in carp (Kuehl et al. 1987);

elimination $t_{1/2} = 3.0$ d, 0.27 d (rainbow trout, exposed to 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988);

elimination $t_{1/2} = 0.8$ d for lactating cows (Olling et al. 1991);

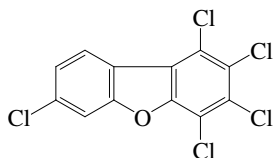
$t_{1/2} > 7$ d for PBO treated goldfish, $t_{1/2} = 3.1$ d for control fish in 120-h exposure studies (Sijm et al. 1993)

elimination $t_{1/2} = 111$ d from soft-shell clam (Brown 1994).

biological $t_{1/2} = 58$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

Depuration $t_{1/2} = 26$ d for newly contaminated oysters, and $t_{1/2} = 36$ d for chronically contaminated oysters (Gardinali et al. 2004)

9.1.1.18 1,2,3,4,7-Pentachlorodibenzofuran



Common Name: 1,2,3,4,7-Pentachlorodibenzofuran

Synonym: 1,2,3,4,7-PCDF

Chemical Name: 1,2,3,4,7-pentachlorodibenzofuron

CAS Registry No: 83704-48-7

Molecular Formula: $C_{12}H_3Cl_5O$, $C_6Cl_4OC_6H_3Cl$

Molecular Weight: 340.418

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

281.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

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

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0179 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.00745; 0.0179 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.43×10^{-5} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

2.09×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 34.22 - 6088/(T/K) - 7.865 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.905×10^{-5} , 1.202×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

2.24 (calculated-SOFA model, Govers & Krop 1998)

1.35; 2.24 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.53 (shake flask/slow stirring-GC/MS, mixture of fly-ash extract, Sijm et al. 1989)

6.89 (calculated-SOFA model, Govers & Krop 1998)

6.45; 6.89 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.80 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.13; 4.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

7.89 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

8.06; 7.89 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (3.6 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991) $k_{OH} = (1.0 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 3.6\text{--}15 \text{ d}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991) $k_{OH}(\text{calc}) = (0.5 - 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 15\text{--}29 \text{ d}$ for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2): $k_1 = 68 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 120-h exposure: control fish, Sijm et al. 1993) $k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993) $k_2 > 0.5$, $< 1.7 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991)
calculated tropospheric lifetime to be 15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995)

Surface water:

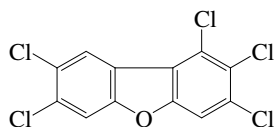
Ground water:

Sediment:

Soil:

Biota: $t_{1/2} < 1.4 \text{ d}$ for PBO treated goldfish and $t_{1/2} < 0.4 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.19 1,2,3,7,8-Pentachlorodibenzofuran



Common Name: 1,2,3,7,8-Pentachlorodibenzofuran

Synonym:

Chemical Name:

CAS Registry No: 57117-41-6

Molecular Formula: $C_{12}H_3Cl_5O$, $C_6HCl_3OC_6H_2Cl_2$

Molecular Weight: 340.418

Melting Point ($^{\circ}C$):

225–227 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

464.7 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

281.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.6 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

128.978 (Rordorf 1989)

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

42.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

85 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0108 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.794 - 2223/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

0.0679; 0.0108 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.27×10^{-5} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

2.3×10^{-7} , 1.5×10^{-5} , 4.0×10^{-4} , 8.0×10^{-3} , 0.11 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

6.17×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

2.40×10^{-4} ; 2.35×10^{-7} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.67 - 5750/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.23 - 3529/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.084×10^{-6} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

1.084×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56$ J/mol K, Mader & Pankow 2003)

$\log (P_L/mmHg) = 34.15 - 6081/(T/K) - 7.865 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.70×10^{-3} , 6.17×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ or as indicated and reported temperature dependence equations):

1.91 (calculated-SOFA model, Govers & Krop 1998)

$\log (H/(Pa \cdot m^3/mol)) = 7.44 - 1306/(T/K)$ (Passivirta et al. 1999)

1.35; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 6.79 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)
 6.99 (calculated-SOFA model, Govers & Krop 1998)
 7.07 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
 6.47; 6.99 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 11.4 (7°C, GC retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log K_B :

- 3.38 (guppy, Opperhuizen et al. 1986)
 3.84, 3.61 (gold fish: treated with metabolic inhibitor PBO, control fish, 120-h exposure, Sijm et al. 1993)
 4.84 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.12; 4.84 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

- 7.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 8.03 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 8.11; 8.03 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution, $t_{1/2} = 10.0$ h for native congener (Tysklind & Rappe 1991)

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

$k_{OH}(\text{calc}) = 2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.0 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 3.6–15 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.5 - 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 98, 252 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}, 174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_5 CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0126 \text{ d}^{-1}$ with a biological $t_{1/2} = 24$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be 15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995);

suggested $t_{1/2} = 660$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2} = 13200$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Ground water:

Sediment: $t_{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

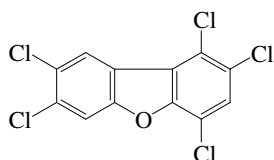
Soil: $t_{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: elimination $t_{1/2} = 3.3$ –3.5 d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);

$t_{1/2} > 7$ d for PBO treated goldfish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2} = 24$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.20 1,2,4,7,8-Pentachlorodibenzofuran



Common Name: 1,2,4,7,8-Pentachlorodibenzofuran

Synonym: 1,2,4,7,8-PeCDF

Chemical Name: 1,2,4,7,8-pentachlorodibenzofuran

CAS Registry No: 83704-51-2

Molecular Formula: $C_{12}H_3Cl_5O$, $C_6HCl_3OC_6H_2Cl_2$

Molecular Weight: 340.418

Melting Point ($^{\circ}C$):

236–238 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

464.7 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

281.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

128.442 (Rordorf 1989)

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

42.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

89 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00179 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.00618; 0.00179 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.0×10^{-7} , 1.1×10^{-5} , 3.4×10^{-4} , 6.7×10^{-3} , 0.091 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

8.92×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

2.34×10^{-5} , 8.91×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log(P_L/mmHg) = 34.28 - 6082/(T/K) - 7.865 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.62 (calculated-SOFA model, Govers & Krop 1998)

1.35; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.26 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)

6.87 (calculated-SOFA model, Govers & Krop 1998)

6.40; 6.87 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, log BCF or log K_B :

- 3.02 (gold fish: treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
 4.85 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.15; 4.85 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

- 7.86 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.96; 7.86 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: $t_{1/2} = 48.5$ d on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

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

$k_{OH}(\text{calc}) = (1.8 - 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.0 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 3.6–15 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.5 - 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 63, 77 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, > 1.3 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}, 174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_5 CDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated tropospheric lifetime $\tau = 15\text{--}29$ d for the gas-phase reaction with OH radical at room temp. (Kwok et al. 1995);

suggested $t_{1/2} = 660$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: suggested $t_{1/2} = 13200$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000)

Ground water:

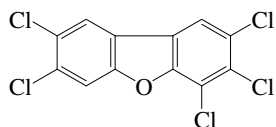
Sediment: suggested $t_{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: elimination $t_{1/2} = 3.3\text{--}3.5$ d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);

$t_{1/2} > 7$ d for metabolic inhibitor PBO treated gold fish and $t_{1/2} < 1.5$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.21 2,3,4,7,8-Pentachlorodibenzofuran



Common Name: 2,3,4,7,8-Pentachlorodibenzofuran

Synonym: 2,3,4,7,8-PCDF

Chemical Name: 2,3,4,7,8-pentachlorodibenzofuran

CAS Registry No: 57117-31-4

Molecular Formula: $C_{12}H_3Cl_5O$, $C_6H_2Cl_2OC_6HCl_3$

Molecular Weight: 340.418

Melting Point ($^{\circ}C$):

196–196.5 (Kuroki et al. 1984, Rordorf 1989)

Boiling Point ($^{\circ}C$):

464.7 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

281.2 (calculated-Le Bas method at normal boiling point)

212.3 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.6 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

130.43 (Rordorf 1989)

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

42.4 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

90 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.0208 (calculated-assuming $\Delta S_{fus} = 56\ J/mol\ K$ and $mp = 196.5^{\circ}C$)

0.00196 (calculated- ΔS_{fus} and mp , Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.000515 (calculated-QSAR, Fiedler & Schramm 1990)

0.000236 ($22.7^{\circ}C$, generator column-GC/MS, Friesen et al. 1990)

0.00015 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.0115; 7.11×10^{-3} (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 1.076 - 2218/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

0.00481; 0.00711 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.17×10^{-5} (supercooled liquid P_L -GC-RT correlation, Eitzer & Hites 1988, 1991)

2.43×10^{-5} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

3.5×10^{-7} , 2.1×10^{-5} , 6.7×10^{-4} , 1.4×10^{-2} , 0.19 ($25, 50, 75, 100, 125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

1.74×10^{-5} (supercooled liquid P_L , Falconer & Bidleman 1994; quoted, Kaupp & McLachlan 1999)

1.53×10^{-4} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)

1.95×10^{-5} ; 5.50×10^{-5} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

1.91×10^{-4} ; 3.74×10^{-7} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.62 - 5677/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.90 - 3462/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

- 6.53×10^{-6} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)
 3.20×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56$ J/mol K, Mader & Pankow 2003)
 $\log (P_L/\text{mmHg}) = 33.99 - 6084/(T/K) - 7.865 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 1.15×10^{-5} , 5.50×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations):

- 0.505 (calculated-P/C with selected values)
 0.575; 2.57 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log (H/(\text{Pa m}^3/\text{mol})) = 6.82 - 1244/(T/K)$ (Passivirta et al. 1999)
 1.29; 2.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 6.92 (shake flask/slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989)
 7.82 (calculated-QSAR, Fiedler & Schramm 1990)
 7.60 (calculated, Broman et al. 1991)
 6.92 (recommended, Hansch et al. 1995)
 7.11 (calculated-SOFA model, Govers & Krop 1998)
 7.11, 6.90 (quoted, calculated-solubility $\log S_L$ and regression from lit. $\log K_{ow}$, Passivirta et al. 1999)
 6.757 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 6.56; 7.11 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.09 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
 11.52 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

- 3.70 (guppy, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990)
 5.14; 4.92 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 5.14; 5.15; 5.38 (guppies, 21-d exposure, lipid weight basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 5.14; 4.79 (lipid wt basis, quoted exptl.; quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 5.62; 5.92, 6.92 (fish 5% lipid: wet wt basis; fish 10% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
 6.42, 5.88 (fish muscle $\log BCF_L$ calculated from water, sediment, Wu et al. 2001)
 5.08; 4.79 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Bioaccumulation Factor, BAF:

- 1.44, 1.33 (rainbow trout, concn in food: 0.82, 9.01 ng/g, Muir et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.59 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 7.40 (calculated, Broman et al. 1991)
 6.60, 6.92 (calculated- K_{ow} , Kollig 1993)
 8.20 (calculated-SOFA model, sediment/water, Govers & Krop 1998)
 8.30; 8.20 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

- Photolysis: photolytic degradation $t_{1/2} = 3.5$ h of PCDD in extract of fly-ash in tetradecane solution for native congener and $t_{1/2} = 3.1$ h for ^{13}C -labelled congener (Tysklind & Rappe 1991)
 $t_{1/2} = 55.0$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Hydrolysis:

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

$k_{OH}(\text{calc}) = (1.7 - 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.0 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 3.6\text{--}15 \text{ d}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.5 - 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 15\text{--}29 \text{ d}$ for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

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

$k_2 = 0.0027 \text{ d}^{-1}$ (carp, calculated from data reported by Kuehl et al. 1987, Sijm et al. 1990)

$k_1 = 400 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.079 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1986)

$k_2 = 0.0064 \text{ d}^{-1}$ (liver of female rat, Van den Berg et al. 1989)

$k_2 = -2.1 \times 10^{-2}$, $1.5 \times 10^{-2} \text{ d}^{-1}$ (rainbow trout, 2 to 21 d exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1990)

$k_2 = 10.1 \times 10^{-3} \text{ d}^{-1}$ and $k_2 = 8.10 \times 10^{-3} \text{ d}^{-1}$; $k_2 = 12.6 \times 10^{-3} \text{ d}^{-1}$ and $k_2 = 11.4 \times 10^{-3} \text{ d}^{-1}$ (rainbow trout, 0–140 d and 0–180 d exposure at 0.82 ng/g PCDF concn.; 0–140 d and 0–180 d exposure at 9.01 ng/g PCDF concn., Muir et al. 1990)

$k_1 = 105$, $561 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.11$, $< 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0081 \text{ d}^{-1}$ with a biological $t_{1/2} = 36 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 1012 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.044 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be 15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995);

$t_{1/2} = 660 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolytic $t_{1/2} = 3.5 \text{ h}$ in the extract from fly-ash in tetradecane solution, for native congener and $t_{1/2} = 3.1 \text{ h}$ for ^{13}C labelled congener (Tysklind & Rappe 1991)

$t_{1/2} = 13200 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{1/2} = 60 \text{ yr}$ (Geyer et al. 2000)

degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ in sediment for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 550\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50 \text{ yr}$ (estimated, Suzuki et al. 2000);

$t_{1/2} = 550\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2} = 108 \text{ d}$ in the liver of female rats (Van den Berg et al. 1989);

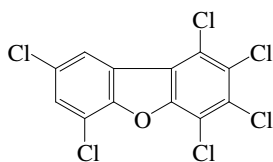
$t_{1/2} = 69 \text{ d}$ in rainbow trout at the 0.82 ng/g exposure concentration from 0–140 d data, $t_{1/2} = 61 \text{ d}$ at 9.0 ng/g exposure concentration from 0–180 d data; $t_{1/2} = 65 \text{ d}$ in whole body rainbow trout with 31-d dietary exposure (Muir et al. 1990);

elimination $t_{1/2} = 48.5 \text{ d}$ for lactating cows (Olling et al. 1991);

$t_{1/2} = 6.1 \text{ d}$ for PBO treated goldfish and $t_{1/2} > 7 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2} = 49 \text{ d}$ in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.22 1,2,3,4,6,8-Hexachlorodibenzofuran



Common Name: 1,2,3,4,6,8-Hexachlorodibenzofuran

Synonym: 1,2,3,4,6,8-HxCDF

Chemical Name: 1,2,3,4,6,8-Hexachlorodibenzofuran

CAS Registry No: 69698-60-8

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6H_2Cl_2OC_6Cl_4$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

233.5–234 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.049 (Rordorf 1989)

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

48.1 (Rordorf 1989; quod, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

95 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F :

0.000332 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

6.08×10^{-3} (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.839 - 2520/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

2.48×10^{-3} , 5.08×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.9×10^{-8} , 2.1×10^{-6} , 8.1×10^{-5} , 1.9×10^{-3} , 0.031 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.67×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

1.74×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

9.39×10^{-5} ; 4.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.84 - 6057/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.88 - 3540/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

5.13×10^{-6} , 1.74×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log (P_L/mmHg) = 32.06 - 6015/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.023 (calculated-SOFA model, Govers & Krop 1998)

$\log (H/(Pa \cdot m^3/mol)) = 7.04 - 1020/(T/K)$ (Passivirta et al. 1999)

1.26; 1.012 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 7.31 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.58 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$ s, Passivirta et al. 1999)
 6.78; 7.31 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

- 4.66 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 4.96; 4.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 8.47 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 8.72; 8.47 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: $t_{1/2} = 59.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Hydrolysis:

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

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

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

$k_1 = 168 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_6\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

suggested $t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_{1/2} = 28\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000);

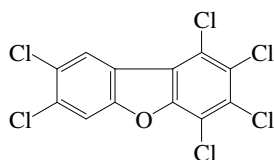
suggested $t_{1/2} = 450\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 450\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} > 7$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993)

9.1.1.23 1,2,3,4,7,8-Hexachlorodibenzofuran



Common Name: 1,2,3,4,7,8-Hexachlorodibenzofuran

Synonym: 1,2,3,4,7,8-HxCDF

Chemical Name: 1,2,3,4,7,8-Hexachlorodibenzofuran

CAS Registry No: 70658-26-9

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6H_2Cl_2OC_6Cl_4$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

225.5–226.5 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.5 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.397 (Rordorf 1989)

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

48.1 (Rordorf 1989; quod, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

96 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F :

0.0107 (calculated-assuming $\Delta S_{fus} = 56\ J/mol\ K$ and $mp = 226^{\circ}C$)

0.000402 (calculated- ΔS_{fus} and mp , Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

8.25×10^{-6} ($22.7^{\circ}C$, generator column-GC/MS, Friesen et al. 1990)

7.30×10^{-6} (computed-expert system SPARC, Kollig 1995)

8.2×10^{-6} , 1.13×10^{-6} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

8.01×10^{-4} ; 2.65×10^{-3} (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.913 - 2516/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.64×10^{-3} , 2.65×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

8.093×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988; quoted, Della Site 1997)

3.2×10^{-8} , 2.4×10^{-6} , 9.3×10^{-5} , 2.2×10^{-3} , 0.036 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.85×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989; quoted, Della Site 1997)

8.90×10^{-8} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

3.09×10^{-6} (supercooled liquid P_L , Falconer & Bidleman 1994;)

8.67×10^{-8} (computed-expert system SPARC, Kollig 1995)

8.41×10^{-8} , 3.68×10^{-8} (P_s solid vapor pressure calculated from reported P_L , Della Site 1997)

6.05×10^{-5} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)
 5.62×10^{-6} ; 1.38×10^{-5} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 2.87×10^{-8} ; 7.13×10^{-5} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F , Passivirta et al. 1999)
 $\log (P_s/Pa) = 12.85 - 6077/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/Pa) = 7.81 - 3564/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P_L/\text{mmHg}) = 32.14 - 6106/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 3.24×10^{-6} , 1.38×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

1.454 (calculated-P/C with selected values)
 4.26 (computed-expert system SPARC, Kollig 1995)
 2.63; 1.91 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 6.90 - 1048/(T/K)$ (Passivirta et al. 1999)
 1.26; 1.905 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

7.70 (calculated, Broman et al. 1991)
 7.86 (computed-expert system SPARC, Kollig 1995)
 7.53 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.54 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$, Passivirta et al. 1999)
 7.184 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 6.92; 7.53 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

10.64 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
 11.98 (7°C , GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log \text{BCF}$:

4.91; 4.40 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.91; 4.99; 5.04 (guppies, 21-d exposure, lipid weight basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.57 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.90, 5.26 (fish muscle $\log \text{BCF}_L$ calculated from water, sediment, Wu et al. 2001)
 4.88; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

7.40 (calculated, Broman et al. 1991)
 7.54 (computed-expert system SPARC, Kollig 1995)
 8.83; 8.80 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 8.95; 8.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: photolytic $t_{1/2} = 5.5$ h of the PCDD in extract of fly ash in tetradecane solution for native congener (Tysklind & Rappe 1991).

Hydrolysis:

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

$k_{O_3}(\text{aq.}) = 7.28 \times 10^4 \text{ L} \cdot \text{g}^{-1} \cdot \text{min}^{-1}$, oxidative degradation rate constant of water dissolved PDCF by ozone under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}} = (0.7\text{--}2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a hexa-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 5.9–22 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

Biodegradation:

Biotransformation:

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

$k_1 = 100, 439 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.31, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P₅CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0126 \text{ d}^{-1}$ with a biological $t_{1/2} = 24 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 879 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.087 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 28\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 600\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50 \text{ yr}$ (estimated, Suzuki et al. 2000);

$t_{1/2} = 600\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

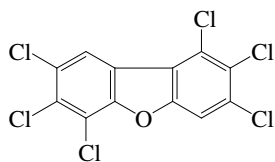
Biota: $t_{1/2} \sim 336 \text{ d}$ in carp (Kuehl et al. 1987);

elimination $t_{1/2} = 48.5 \text{ d}$ from lactating cows (Olling et al. 1991);

$t_{1/2} = 2.2 \text{ d}$ for PBO treated goldfish and $t_{1/2} > 7 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2} = 24 \text{ d}$ in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.24 1,2,3,6,7,8-Hexachlorodibenzofuran



Common Name: 1,2,3,6,7,8-Hexachlorodibenzofuran

Synonym:

Chemical Name: 1,2,3,6,7,8-hexachlorodibenzofuran

CAS Registry No: 57117-44-9

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

232–234 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.1 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.083 (Rordorf 1989)

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

48.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

95 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.000358 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00226 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.125 - 2515/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.56×10^{-3} , 2.26×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

7.33×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

2.9×10^{-8} , 2.1×10^{-6} , 8.2×10^{-5} , 2.0×10^{-3} , 0.031 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.20×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

6.91×10^{-5} ; 2.47×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.87 - 6101/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.91 - 3954/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P_L/mmHg) = 32.12 - 6108/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

3.09×10^{-6} , 1.20×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.91 (calculated-SOFA model, Govers & Krop 1998)

$\log (H/(Pa \cdot m^3/mol)) = 7.79 - 1439/(T/K)$, (Passivirta et al. 1999)

1.26; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 7.60 (calculated, Broman et al. 1991)
 7.57 (calculated-SOFA model, Govers & Krop 1998)
 7.96 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
 7.196 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 6.93; 7.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.0 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.95; 4.49 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.95, 5.15; 5.24 (guppies, 21-d exposure, lipid weight basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.58 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.51 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)
 4.87; 4.58 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.40 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 8.85 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 8.97; 8.85 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: photolytic $t_{1/2} = 5.9$ h in extract of fly-ash and in tetradecane solution for native congener (Tysklind & Rappe 1991);

$t_{1/2} = 74.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

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

$k_{OH}(\text{calc}) = (1.3 - 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 103, 460 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.26, < 0.1 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0138 \text{ d}^{-1}$ with a biological $t_{1/2} = 22$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 1310 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.078 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Ground water:

Sediment: $t_{1/2} = 700000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

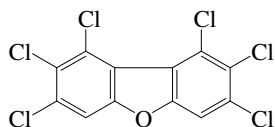
Soil: $t_{1/2} = 700000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: elimination $t_{1/2} = 73$ –156 d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);

$t_{1/2} = 2.7$ d for PBO treated goldfish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2} = 22$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994).

9.1.1.25 1,2,3,7,8,9-Hexachlorodibenzofuran



Common Name: 1,2,3,7,8,9-Hexachlorodibenzofuran

Synonym: 1,2,3,7,8,9-HxCDF

Chemical Name: 1,2,3,7,8,9-hexachlorodibenzofuran

CAS Registry No: 72918-21-9

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

246–249 (Rordorf 1989)

230 (calculated, Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

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

Entropy of Fusion, ΔS_{fus} (J/mol K):

96 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.00036 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.000859 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.892 - 2526/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.06×10^{-3} , 8.59×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.99×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988, 1991)

4.31×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

3.88×10^{-5} (corrected, supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)

2.24×10^{-6} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

4.01×10^{-5} ; 1.44×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.91 - 6185/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.90 - 3625/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P_L/mmHg) = 31.92 - 6114/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

2.09×10^{-6} , 2.24×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.955 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa \cdot m^3/mol)] = 7.01 - 1136/(T/K)$ (Passivirta et al. 1999)

1.29; 0.955 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.00 (calculated, Broman et al. 1991)

7.76 (calculated-SOFA model, Govers & Krop 1998)

- 7.57 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
 7.125 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 7.07; 7.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.17 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.71 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.04 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)
 4.77; 4.71 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 9.08 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 9.19; 9.08 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution: $t_{1/2} = 2.2$ h for native congener and $t_{1/2} = 3.6$ h for ^{13}C -labelled congener (Tysklind & Rappe 1991);
 $t_{1/2} = 78.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

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

$k_{OH}(\text{calc}) = (1.3 - 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_2 = 0.01651 \text{ d}^{-1}$ with a biological $t_{1/2} = 18$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 1101 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.103 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

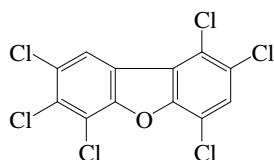
Ground water:

Sediment: $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: biological $t_{1/2} = 18$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.26 1,2,4,6,7,8-Hexachlorodibenzofuran



Common Name: 1,2,4,6,7,8-Hexachlorodibenzofuran

Synonym: 1,2,4,6,7,8-HxCDF

Chemical Name: 1,2,4,6,7,8-hexachlorodibenzofuran

CAS Registry No: 67562-40-7

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

221–222 (Kuroki et al. 1986; Rordorf 1989; Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.593 (Rordorf 1989)

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

48.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

97 (Rordorf 1989; Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.000483 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

0.00451 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.944 - 2512/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

2.26×10^{-3} , 4.51×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.5×10^{-8} , 2.6×10^{-6} , 1.0×10^{-4} , 2.4×10^{-3} , 0.040 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

1.35×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

9.39×10^{-5} ; 4.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.81 - 6006/(T/K)$, (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.74 - 3497/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

4.47×10^{-6} , 2.35×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log (P_L/mmHg) = 32.31 - 6108/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

1.072 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa\ m^3/mol)] = 6.80 - 985/(T/K)$, (Passivirta et al. 1999)

1.26; 1.072 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 7.38 (calculated-SOFA model, Govers & Krop 1998)
- 7.51 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 6.83; 7.38 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.66 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 4.94; 4.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 8.58 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 8.78; 8.58 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: $t_{1/2} = 58.2$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

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

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 345, 293 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.10, > 2.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 170 \text{ L kg}^{-1} \text{ d}^{-1}$, $369 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_6\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 1101 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.103 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

suggested $t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: suggested $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

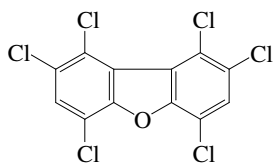
Ground water:

Sediment: suggested $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: $t_{1/2} > 7$ d for PBO treated goldfish and $t_{1/2} < 0.3$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.27 1,2,4,6,8,9-Hexachlorodibenzofuran



Common Name: 1,2,4,6,8,9-Hexachlorodibenzofuran

Synonym: 1,2,3,4,8,9-HxCDF

Chemical Name: 1,2,4,6,8,9-hexachlorodibenzofuran

CAS Registry No: 69698-59-5

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

246–248 (Kuroki et al. 1984; Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

487.7 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

136.462 (Rordorf 1989)

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

48.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

93 (Rordorf 1989; Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.000245 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

0.00305 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.892 - 2526/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.92×10^{-3} , 3.05×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.4×10^{-8} , 1.7×10^{-6} , 6.4×10^{-5} , 1.5×10^{-3} , 0.024 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

9.22×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

3.55×10^{-6} supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

7.96×10^{-5} ; 1.95×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.89 - 6137/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.08 - 3629/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

3.89×10^{-6} , 3.55×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log (P_L/mmHg) = 32.22 - 6105/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.417 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa \cdot m^3/mol)] = 7.40 - 1117/(T/K)$ (Passivirta et al. 1999)

1.26; 0.417 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 7.43 (calculated-SOFA model, Govers & Krop 1998)
- 7.65 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 6.87; 7.43 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.84 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 4.91; 4.84 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 8.58 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 8.86; 8.58 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: $t_{1/2} = 82.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

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

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 170 \text{ L kg}^{-1} \text{ d}^{-1}$, $369 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_6\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 > 2.0 \text{ d}^{-1}$ (120-h exposure: metabolic inhibitor PBO-treated goldfish, Sijm et al. 1993)

$k_1 = 1101 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.103 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

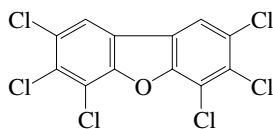
Ground water:

Sediment: $t_{1/2} = 150000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{1/2} = 150000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: $t_{1/2} < 0.3$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.28 2,3,4,6,7,8-Hexachlorodibenzofuran



Common Name: 2,3,4,6,7,8-Hexachlorodibenzofuran

Synonym: 2,3,4,6,7,8-HCDF

Chemical Name: 2,3,4,6,7,8-hexachlorodibenzofuran

CAS Registry No: 60851-34-5

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

239–240 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.7 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

136.794 (Rordorf 1989)

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

48.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

94 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25 $^{\circ}C$, F:

0.000276 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00156 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.787 - 2527/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.24×10^{-3} , 1.56×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations):

4.99×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988, 1991)

5.82×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

3.88×10^{-5} (corrected, supercooled liquid P_L , in Eitzer & Hites 1988, Eitzer & Hites 1998)

2.6×10^{-8} , 1.9×10^{-6} , 7.3×10^{-5} , 1.7×10^{-3} , 0.028 (25, 50, 75, 100, 125 $^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.59×10^{-6} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

5.54×10^{-5} ; 1.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.91 - 6175/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.00 - 3651/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P_L/mmHg) = 31.99 - 6108/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

2.45×10^{-6} , 7.59×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa·m³/mol or as indicated and reported temperature dependence equations):

1.78 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa \cdot m^3/mol)] = 7.21 - 1124/(T/K)$ (Passivirta et al. 1999)

1.26; 1.78 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 7.0 (calculated, Broman et al. 1991)
- 7.65 (calculated-SOFA model, Govers & Krop 1998)
- 7.62 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 6.937 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.01; 7.65 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 12.10 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log K_B :

- 4.88 (goldfish, 120-h exposure studies, Sijm et al. 1993)
- 4.99; 4.94; 5.02 (guppies, 21-d exposure, lipid weight basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
- 4.59 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 5.51 (fish muscle log BCF_L calculated from water, Wu et al. 2001)
- 4.81; 4.59 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

- 6.80 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 8.96 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 9.10; 8.96 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

- Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution: $t_{1/2} = 2.8$ h for native congener (Tysklind & Rappe 1991);
- $t_{1/2} = 70.7$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

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

- $k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

- $k_1 = 267 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1 \text{ d}^{-1}$ (goldfish after 120-h exposure: control fish, Sijm et al. 1993)
- $k_2 = 0.36$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P₅CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- $k_2 = 0.0119 \text{ d}^{-1}$ with a biological $t_{1/2} = 25$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

- Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

- Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

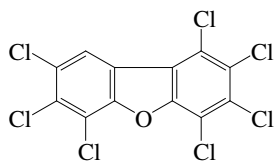
Ground water:

- Sediment: $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

- Soil: $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

- Biota: $t_{1/2} = 1.9$ d for PBO treated goldfish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993).
- biological $t_{1/2} = 25$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.29 1,2,3,4,6,7,8-Heptachlorodibenzofuran



Common Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran

Synonym: 1,2,3,4,6,7,8-HCDF

Chemical Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran

CAS Registry No: 67562-39-4

Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$

Molecular Weight: 409.308

Melting Point ($^{\circ}C$):

236–237 (Kuroki et al. 1984; Rordorf 1989; Della Site 1997)

Boiling Point ($^{\circ}C$):

507.2 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

323.0 (calculated-Le Bas method at normal boiling point)

238.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

87.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

144.642 (Rordorf 1989)

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

53.9 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

106 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.000122 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.35×10^{-6} ($22.7^{\circ}C$, generator column-GC/MS, Friesen et al. 1990)

1.08×10^{-5} (calculated-QSAR, Fiedler & Schramm 1990)

9.50×10^{-7} (computed-expert system SPARC, Kollig 1995)

1.26×10^{-7} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.63×10^{-4} ; 7.11×10^{-4} (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.917 - 2812/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

4.92×10^{-4} , 7.11×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.24×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988, 1991; quoted, Della Site 1997)

1.93×10^{-6} (supercooled liquid P_L GC-RT correlation, Eitzer & Hites 1989; quoted, Della Site 1997)

4.7×10^{-9} , 4.3×10^{-7} , 2.0×10^{-5} , 5.8×10^{-4} , 1.1×10^{-2} (25 , 50 , 75 , 100 , $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

5.10×10^{-8} (gas saturation method, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

8.70×10^{-9} (computed-expert system SPARC, Kollig 1995)

1.83×10^{-8} , 1.58×10^{-8} (P_s solid vapor pressure calculated from reported P_L , Della Site 1997)

1.84×10^{-5} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)

1.4×10^{-6} ; 2.51×10^{-6} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

5.54×10^{-5} ; 6.76×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.98 - 6302/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/Pa) = 7.45 - 3486/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P_L/mmHg) = 30.03 - 6090/(T/K) - 6.798 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 9.33×10^{-7} , 2.51×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \text{ m}^3/\text{mol}$ at 25°C):

3.80 (computed-expert system SPARC, Kollig 1995)
 3.47; 1.41 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(Pa \text{ m}^3/\text{mol})] = 6.53 - 674/(T/K)$ (Passivirta et al. 1999)
 1.41; 1.41 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.92 (shake flask/slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989a)
 9.25 (calculated-QSAR, Friedler & Schramm 1990)
 7.90 (quoted, Loonen et al. 1991)
 8.10 (calculated, Broman et al. 1991)
 7.92 (recommended, Hansch et al. 1995)
 8.52 (computed-expert system SPARC, Kollig 1995)
 8.01 (calculated-SOFA model, Govers & Krop 1998)
 8.07 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{ow}$, Passivirta et al. 1999)
 7.477 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 7.37; 8.00 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

12.06 (7°C , GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

4.46; 4.08 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.46; 4.60; 4.63 (guppy, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.46; 4.26 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 6.62; 6.92 (wet wt basis, fish 5% lipid, 10% lipid, Geyer et al. 2000)
 5.89, 6.03 (fish muscle $\log BCF_L$ calculated from water, sediment, Wu et al. 2001)
 4.51; 4.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{oc}$:

6.37 (organic carbon, calculated-QSAR, Friedler & Schramm 1990)
 6.00 (organic carbon, calculated, Broman et al. 1991)
 7.90 (calculated, Broman et al. 1991)
 8.20 (computed- K_{ow} , Kollig 1995)
 9.07; 9.48 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 9.64; 9.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: photolytic degradation $t_{1/2} = 9.8 \text{ h}$ with extract of fly-ash and in tetradecane solution for native congener and $t_{1/2} = 3.7 \text{ h}$ for ^{13}C -labelled congener (Tysklind & Rappe 1991).

$t_{1/2} = 84.5 \text{ h}$ on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Hydrolysis:

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

$k_{O_3}(aq.) = 1.08 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$, oxidative degradation rate constant of water dissolved PCDF by ozone under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{OH}(calc) = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.5 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 17\text{--}31 \text{ d}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

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

$k_1 = 42, 61 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.43, 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 42 \text{ L kg}^{-1} \text{ d}^{-1}$, $61 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P₅CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0084 \text{ d}^{-1}$ with a biological $t_{1/2} = 36 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 524 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.127 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF with OH radicals to be 17–31 d (Atkinson 1991);

$t_{1/2} = 3200 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 64\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{1/2} = 36 \text{ yr}$ (Geyer et al. 2000)

degradation $t_{1/2} = 2\text{--}200 \text{ yr}$ for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 350\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50 \text{ yr}$ (estimated, Suzuki et al. 2000);

$t_{1/2} = 350\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

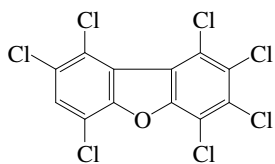
Biota: depuration $t_{1/2} > 336 \text{ d}$ for carp in Lake Superior water (Kuehl et al. 1987);

elimination $t_{1/2} = 33.9 \text{ d}$ from lactating cow (Olling et al. 1991);

$t_{1/2} = 1.6 \text{ d}$ for PBO treated goldfish and $t_{1/2} = 6.8 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

biological $t_{1/2} = 37 \text{ d}$ in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.30 1,2,3,4,6,8,9-Heptachlorodibenzofuran



Common Name: 1,2,3,4,6,8,9-Heptachlorodibenzofuran

Synonym: 1,2,3,4,6,8,9-HpCDF

Chemical Name: 1,2,3,4,6,8,9-Heptachlorodibenzofuran

CAS Registry No: 69698-58-4

Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$

Molecular Weight: 409.308

Melting Point ($^{\circ}C$):

211–212 (Kuroki et al. 1984; Rordorf 1989; Della Site 1997)

Boiling Point ($^{\circ}C$):

507.2 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

323.0 (calculated-Le Bas method)

238.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

89.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

145.64 (Rordorf 1989)

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

53.9 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

111 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.00021 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

5.65×10^{-4} (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 1.200 - 2861/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

4.19×10^{-4} , 5.65×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

7.7×10^{-9} , 7.2×10^{-7} , 3.6×10^{-5} , 1.0×10^{-3} , 2.0×10^{-2} (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.24×10^{-7} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

1.55×10^{-5} ; 3.57×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 13.03 - 6394/(T/K)$, (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.23 - 3581/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

8.13×10^{-7} , 7.24×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log (P_L/mmHg) = 29.94 - 6089/(T/K) - 6.798 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

5.13 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa \cdot m^3/mol)] = 6.03 - 756/(T/K)$, (Passivirta et al. 1999)

1.45; 5.13 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 8.02 (calculated-SOFA model, Govers & Krop 1998)
 7.91 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$, Passivirta et al. 1999)
 7.43; 8.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

- 4.42 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 4.46; 4.42 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 9.45 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 9.72; 9.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: $t_{1/2} = 85.6$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Hydrolysis:

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

$k_{OH}(\text{calc}) = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.5 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 17–31 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

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

$k_1 = 42 \text{ L kg}^{-1} \text{ d}^{-1}$, $61 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_7\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF with OH radical to be 17–31 d (Atkinson 1991);

suggested $t_{1/2} = 3200$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_{1/2} = 64\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 2\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000);

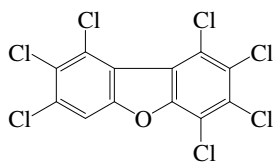
suggested $t_{1/2} = 350\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 350\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Biota:

9.1.1.31 1,2,3,4,7,8,9-Heptachlorodibenzofuran



Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran

Synonym: 1,2,3,4,7,8,9-HCDF

Chemical Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran

CAS Registry No: 55673-89-7

Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$

Molecular Weight: 409.308

Melting Point ($^{\circ}C$):

221–223 (Kuroki et al. 1984)

Boiling Point ($^{\circ}C$):

507.2 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

323.0 (calculated-Le Bas method at normal boiling point)

248.1 (Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.6 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

145.221 (Rordorf 1989)

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

53.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

109 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.000179 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.30×10^{-6} (computed-expert system SPARC, Kollig 1995)

2.58×10^{-4} (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 1.100 - 2819/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

2.83×10^{-4} , 2.58×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.2×10^{-9} , 5.8×10^{-7} , 2.8×10^{-5} , 8.0×10^{-4} , 1.5×10^{-2} (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1987, 1989)

1.305×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988, 1991)

1.011×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

1.27×10^{-9} (computed-expert system SPARC, Kollig 1995)

1.48×10^{-8} , 1.14×10^{-8} (solid vapor pressures calculated from reported P_L , Della Site 1997)

6.61×10^{-7} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

7.87×10^{-6} ; 1.41×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 13.12 - 6547/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.23 - 3581/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P_L/mmHg) = 29.69 - 6089/(T/K) - 6.798 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

5.75×10^{-7} , 6.60×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations):

- 3.85 (computed-expert system SPARC, Kollig 1995)
- 1.0 (calculated-SOFA model, Govers & Krop 1998)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 6.32 - 912/(T/K)$ (Passivirta et al. 1999)
- 1.58; 1.0 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

- 6.90 (calculated, Broman et al. 1991)
- 8.50 (computed-expert system SPARC, Kollig 1995)
- 8.23 (calculated-SOFA model, Govers & Krop 1998)
- 7.99 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$, Passivirta et al. 1999)
- 7.616 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.60; 8.23 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25 °C or as indicated:

- 12.34 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

- 4.32 (calculated-SOFA model, Govers & Krop 1998)
- 5.59 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)
- 4.30; 4.32 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.00 (organic carbon, calculated, Broman et al. 1991)
- 6.70 (calculated, Broman et al. 1991)
- 8.23 (computed- K_{OW} , Kollig 1995)
- 9.78; 9.76 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
- 9.92; 9.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: photolysis $t_{1/2} = 3.3$ h in the extract from fly ash in tetradecane, for ^{13}C labelled congener (Tysklind & Rappe 1991)

$t_{1/2} = 84.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

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

$k_{OH}(\text{calc}) = 0.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.5 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 17–31 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 42 \text{ L kg}^{-1} \text{ d}^{-1}$, $61 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for H_7CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF, with OH radicals to be 17–31 d (Atkinson 1991);

$t_{1/2} = 3200$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 64\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ y for all homologues (estimated, Suzuki et al. 2000);

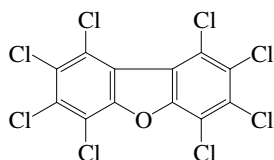
$t_{1/2} = 300\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr (estimated, Suzuki et al. 2000);

$t_{1/2} = 300\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota:

9.1.1.32 Octachlorodibenzofuran



Common Name: Octachlorodibenzofuran

Synonym: OCDF

Chemical Name: octachlorodibenzofuran

CAS Registry No: 39001-02-0

Molecular Formula: $C_6Cl_4OC_6Cl_4$

Molecular Weight: 443.753

Melting Point ($^{\circ}C$):

258–260 (Rordorf 1986,1989)

259 (Ruelle & Kesselring 1997, Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

510 (calculated, Rordorf 1986)

537 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

343.9 (calculated-Le Bas method at normal boiling point)

251.0 (Ruelle & Kesselring 1997, quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

90 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

149.43 (Rordorf 1989)

284.38 (Dickhut et al. 1994)

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

57.5 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

108 (Rordorf 1986,1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.00518 (calculated-assuming $\Delta S_{fus} = 56$ J/mol K and mp = $258^{\circ}C$)

0.000037 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.16×10^{-6} * (extrapolated, generator column-GC, measured range 39.8 – $80^{\circ}C$, Doucette & Andren 1988a)

$S/(mol/L) = 2.77 \times 10^{-14} \exp(0.081 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range 40 – $80^{\circ}C$, Doucette & Andren 1988a)

$\log x = -3264/(T/K) - 2.376$, temp range 40 – $80^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

1.54×10^{-6} (calculated-QSAR, Fiedler & Schramm 1990)

1.37×10^{-7} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

2.33×10^{-4} ; 1.02×10^{-4} (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.5720 - 3008/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -5.0496 - 7455.1/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

1.22×10^{-4} , 1.02×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

5.00×10^{-10} * (gas saturation, Rordorf 1985, 1989)

2.60×10^{-7} (supercooled liquid P_L , GC-RC correlation, Eitzer & Hites 1989)

0.000221* (105.6 °C, average value, gas saturation-GC, measured range 105.6–261.2 °C, Rordorf 1990)
 5.00×10^{-10} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
 1.26×10^{-9} (solid vapor pressure calculated from reported P_L , Delle Site 1997)
 7.08×10^{-7} ; 1.82×10^{-7} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 1.30×10^{-6} ; 4.83×10^{-11} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 13.42 - 7073/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 7.77 - 4068/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P/\text{Pa}) = 16.88937 - 7808.74/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 0.107* (165 °C, Knudsen effusion, measured range 165–195°C, Li et al. 2002)
 $\log (P_L/\text{mmHg}) = 27.96 - 6148/(T/K) - 6.267 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations):

0.10 (estimated, Clark & Mackay 1991)
 1.31; 0.776 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 7.20 - 1060/(T/K)$ (Passivirta et al. 1999)
 2.14; 0.776 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

13.06, 13.22, 13.78; 12.54, 13.37, 13.93 (HPLC-RT correlation, linear regressions; quadratic regressions, Sarna et al. 1984)
 8.78 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
 7.97 (generator column-GC/ECD, Doucette & Andren 1987, 1988b)
 7.90 (HPLC-RT correlation, Doucette & Andren 1988b)
 7.97 (recommended, Hansch et al. 1995)
 8.78; 8.60 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 8.62 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$, Passivirta et al. 1999)
 7.992 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 8.03; 8.60 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

12.84 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

1.613, 0.70 (human fat, calculated-different K_{OWS} , wet weight basis, Geyer et al. 1987)
 1.71, 0.778 (human fat, calculated-different K_{OWS} , lipid basis, Geyer et al. 1987)
 2.77; 3.89 (guppy, wet weight based; lipid weight based, Gobas & Schrap 1990)
 3.90; 4.10; 4.11 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 3.90; 3.88 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 7.48; 7.78 (wet wt basis: fish with 5% lipid, with 10% lipid, Geyer et al. 2000)
 7.61, 7.63 (fish muscle $\log BCF_L$ calculated from water, sediment, Wu et al. 2001)
 3.85; 3.88 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

6.75 (calculated-QSAR, Fiedler & Schramm 1990)
 6.00 (organic carbon, calculated, Broman et al. 1991)
 7.40 (calculated, Broman et al. 1991)
 7.40 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 8.13, 8.48 (calculated- K_{OW} , Kollig 1993)
 10.49; 10.30 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 10.39; 10.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

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

Volatilization:

Photolysis: photolytic $t_{1/2} = 2.1$ h from extract of fly ash in tetradecane solution for native congener (Tysklind & Rappe 1991);

photolysis $k = 2.7 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 260$ min in pure water and $t_{1/2} = 6.3 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 110$ min in 60% acetonitrile/water at 300 nm photochemical reactor; $k = 0.11 \text{ h}^{-1}$ with $t_{1/2} = 6.5$ h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000).

$t_{1/2} = 100.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Hydrolysis:

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

k (oxidative degradation rate constant of water dissolved OCDF by ozone) is $1.05 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 0.39 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = 0.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 39$ d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for OCDF at room temp. (Atkinson 1991)

photodegradation $t_{1/2} = 9$ h for OCDF adsorbed to clean silica gels in a rotary photo-reactor by filtered < 290 nm of light (Koester & Hites 1992)

Biodegradation:

Biotransformation: metabolism half-time 10^7 h (guppy, Clark & Mackay 1991).

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

$k_2 = 0.012 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986)

$k_1 = 824 \text{ d}^{-1}$; $k_2 = 1.40 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

$k_2 = 0.0101 \text{ d}^{-1}$ with a biological $t_{1/2} = 30$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 217 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.174 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for OCDF with OH radicals to be 39 d (Atkinson 1991);

$t_{1/2} = 9600$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis $k = 2.7 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 260$ min in pure water and $k = 6.3 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 110$ min in 60% acetonitrile/water at 300 nm photochemical reactor; $k = 0.11 \text{ h}^{-1}$ with a $t_{1/2} = 6.5$ h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000);

$t_{1/2} = 192000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{1/2} = 29$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 250\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr (estimated, Suzuki et al. 2000);

$t_{1/2} = 250000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: mean biological $t_{1/2} = 7$ d in rainbow trout (Niimi 1986)

$t_{1/2} = 7$ to 12 d in rainbow trout (Niimi & Oliver 1986)

biological $t_{1/2} = 30$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

[illegible]

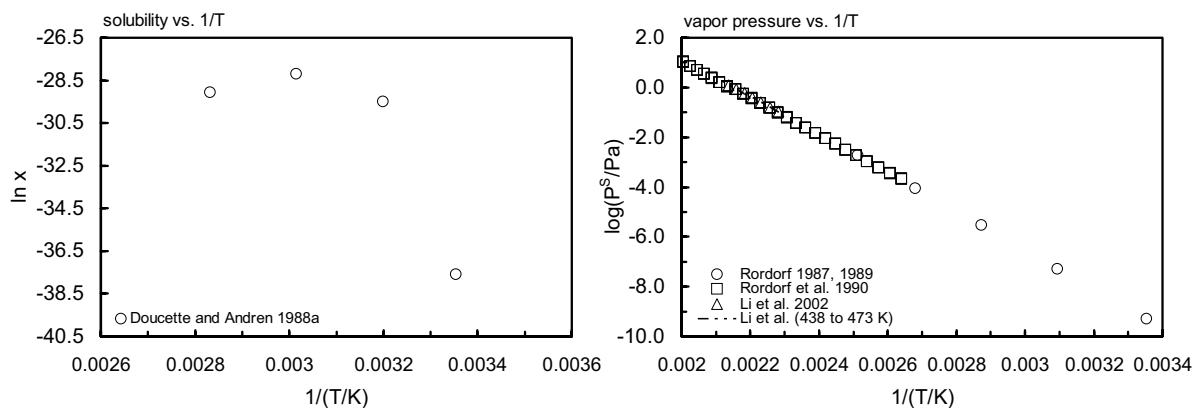


FIGURE 9.1.32.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for octachlorodibenzofuran.

9.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 9.2.1
Summary of physical properties of some chlorinated furans

Compound	CAS no.	Molecular formula	Chlorine no. n	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume V _M cm ³ /mol
Dibenzofuran	132-64-9	C ₁₂ H ₈ O	0	168.191	86.5	287	0.249	176.1
2-Chloro-	51230-49-0	C ₁₂ H ₇ OCl	1	202.637	101.5–102.5	338.2	0.175	197.6
3-Chloro-	25074-67-3	C ₁₂ H ₇ OCl	1	202.637	101–102	338.2	0.178	197.6
2,3-Dichloro-	64126-86-9	C ₁₂ H ₆ OCl ₂	2	237.082	125.5–127	375.0	0.102	218.5
2,7-Dichloro-	73992-98-6	C ₁₂ H ₆ OCl ₂	2	237.082				218.5
2,8-Dichloro-	5409-83-6	C ₁₂ H ₆ OCl ₂	2	237.082	184–185	375	0.0272	218.5
3,6-Dichloro-	94570-83-9	C ₁₂ H ₆ OCl ₂	2	237.082	188	375	0.0252	218.5
2,3,8-Trichloro-	57117-32-5	C ₁₂ H ₅ OCl ₃	3	271.527	189–191	408.4	0.0240	239.4
2,4,6-Trichloro-	58802-14-5	C ₁₂ H ₅ OCl ₃	3	271.527	116–117	408.4	0.126	239.4
2,4,8-Trichloro-	54589-71-8	C ₁₂ H ₅ OCl ₃	3	271.527	154	392.5	0.0542	239.4
1,2,3,4-Tetrachloro-	24478-72-6	C ₁₂ H ₄ OCl ₄	4	305.978	168.5–169	438.3	0.0389	260.3
1,2,3,7-Tetrachloro-	83704-22-7	C ₁₂ H ₄ OCl ₄	4	305.978	167.5–168	438.3	0.0398	260.3
1,2,7,8-Tetrachloro-	58802-20-3	C ₁₂ H ₄ OCl ₄	4	305.978	210–211	438.3	0.0151	260.3
1,3,6,8-Tetrachloro-	71998-72-6	C ₁₂ H ₄ OCl ₄	4	305.978	177–178	438.3	0.0319	260.3
1,3,7,8-Tetrachloro-	57117-35-8	C ₁₂ H ₄ OCl ₄	4	305.978				260.3
1,3,7,9-Tetrachloro-	64650-17-4	C ₁₂ H ₄ OCl ₄	4	305.978	206.5–207.5	438.3	0.0168	260.3
2,3,7,8-Tetrachloro-	51207-31-9	C ₁₂ H ₄ OCl ₄	4	305.978	227	438.3	0.0104	260.3
1,2,3,4,7-Pentachloro-	83704-48-7	C ₁₂ H ₃ OCl ₅	5	340.418				281.2
1,2,3,7,8-Pentachloro-	57117-41-6	C ₁₂ H ₃ OCl ₅	5	340.418	225–227	464.7	0.0107	281.2
1,2,4,7,8-Pentachloro-	83704-51-2	C ₁₂ H ₃ OCl ₅	5	340.418	236–238	464.7	0.00832	281.2
2,3,4,7,8-Pentachloro-	57117-31-4	C ₁₂ H ₃ OCl ₅	5	340.418	196–196.5	464.7	0.0209	281.2
1,2,3,4,6,8-Hexachloro-	69698-60-8	C ₁₂ H ₂ OCl ₆	6	374.863	233.5–234	487.7	0.00895	302.1
1,2,3,4,7,8-Hexachloro-	70658-26-9	C ₁₂ H ₂ OCl ₆	6	374.863	226	487.7	0.107	302.1
1,2,3,4,7,9-Hexachloro-	91538-84-0	C ₁₂ H ₂ OCl ₆	6	374.863	216–217	487.7	0.0132	302.1
1,2,3,6,7,8-Hexachloro-	57117-44-9	C ₁₂ H ₂ OCl ₆	6	374.863	232–234	487.7	0.00910	302.1
1,2,3,7,8,9-Hexachloro-	72918-21-9	C ₁₂ H ₂ OCl ₆	6	374.863	246–249	487.7	0.00656	302.1
1,2,4,6,7,8-Hexachloro-	67562-40-7	C ₁₂ H ₂ OCl ₆	6	374.863	221–222	487.7	0.0118	302.1
1,2,4,6,8,9-Hexachloro-	68698-59-5	C ₁₂ H ₂ OCl ₆	6	374.863	246–248	487.7	0.00664	302.1

Continued

TABLE 9.2.1 (continued)

Compound	CAS no.	Molecular formula	Chlorine no. n	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume V_M cm ³ /mol
2,3,4,6,7,8-Hexachloro-	60851-34-5	C ₁₂ H ₂ OCl ₆	6	374.863	239-240	487.7	0.00786	302.1
1,2,3,4,6,7,8-Heptachloro-	67462-39-4	C ₁₂ HOCl ₇	7	409.308	236-237	507.2	0.00841	323.0
1,2,3,4,6,8,9-Heptachloro-	69698-58-4	C ₁₂ HOCl ₇	7	409.308	211-212	507.2	0.0148	323.0
1,2,3,4,7,8,9-Heptachloro-	55673-89-7	C ₁₂ HOCl ₇	7	409.308	221-223	507.2	0.0117	323.0
Octachlorodibenzofuran	39001-02-0	C ₁₂ OCl ₈	8	443.753	258	537	0.00518	343.9

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

TABLE 9.2.2

Selected physical-chemical properties of some chlorinated furans at 25°C

Compound	Selected properties					log K _{OW}	Henry's law const. H/(Pa·m ³ /mol)
	Vapor pressure		Solubility				
	P ^S /Pa	P _L /Pa	S/(mg/m ³)	C ^S /(mmol/m ³)	C _L /(mmol/m ³)		calculated P/C
Dibenzofuran	0.400	1.606	4750	28.240	114.42	4.27	14.16
2,8-DCDF	0.00039	1.46×10 ⁻²	14.5	0.0612	2.246	5.44	6.377
3,6-DCDF	2.00×10 ⁻⁴	7.94×10 ⁻³					
2,3,8-T ₃ CDF	2.48×10 ⁻⁴	1.03×10 ⁻²					
2,4,6-T ₃ CDF	9.22×10 ⁻⁴	7.29×10 ⁻³					
2,4,8-T ₃ CDF	9.1×10 ⁻⁵	1.68×10 ⁻³					
1,3,7,8-T ₄ CDF	3.51×10 ⁻⁵					6.39	
2,3,7,8-T ₄ CDF	2.00×10 ⁻⁶	1.92×10 ⁻⁴	0.419	1.37×10 ⁻³	0.132	6.53	1.461
2,3,4,7,8-P ₅ CDF	3.50×10 ⁻⁷	1.68×10 ⁻⁵	0.236	6.93×10 ⁻⁴	0.0332	6.5	0.505
1,2,3,4,7,8-H ₆ CDF	3.20×10 ⁻⁸	2.99×10 ⁻⁶	0.00825	2.20×10 ⁻⁵	2.06×10 ⁻³	7.0	1.454
1,2,3,4,6,7,8-H ₇ CDF	4.70×10 ⁻⁹	5.59×10 ⁻⁷	0.00135	3.30×10 ⁻⁶	3.92×10 ⁻⁴	7.4	1.425
OCDF	5.0×10 ⁻¹⁰	9.65×10 ⁻⁸	0.00116	2.61×10 ⁻⁶	5.05×10 ⁻⁵	8.0	0.191

TABLE 9.2.3

Suggested half-life classes of polychlorinated dibenzofurans in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Dibenzofuran	3	4	6	7
2,8-Dichloro-	4	5	7	8
2,3,7,8-Tetrachloro-	4	5	8	9
2,3,4,7,8-Pentachloro-	5	5	8	9
1,2,3,4,6,7,8-Heptachloro-	5	6	8	9
Octachlorodibenzofuran	5	7	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

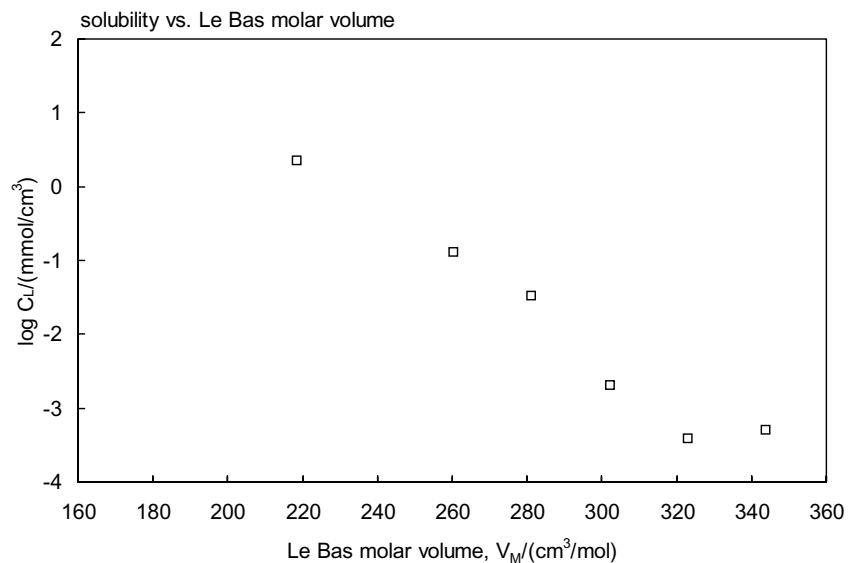


FIGURE 9.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzofurans.

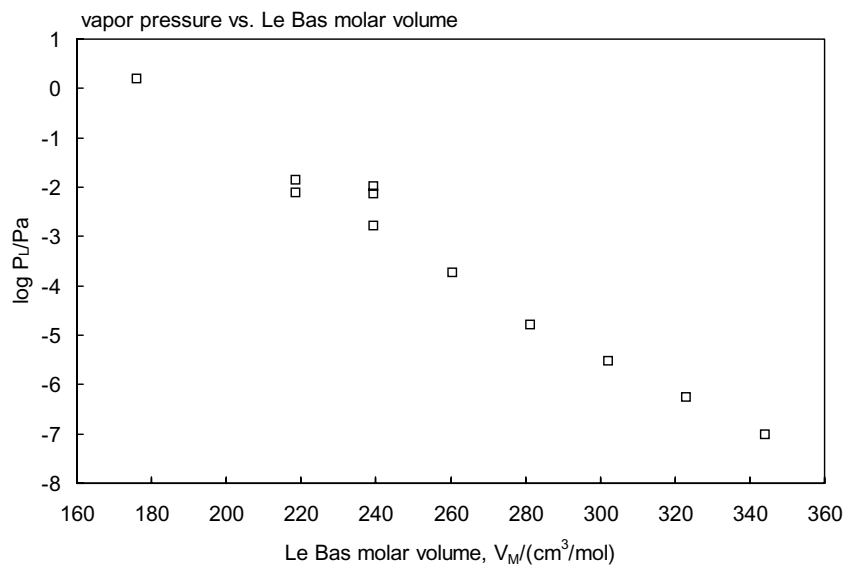


FIGURE 9.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzofurans.

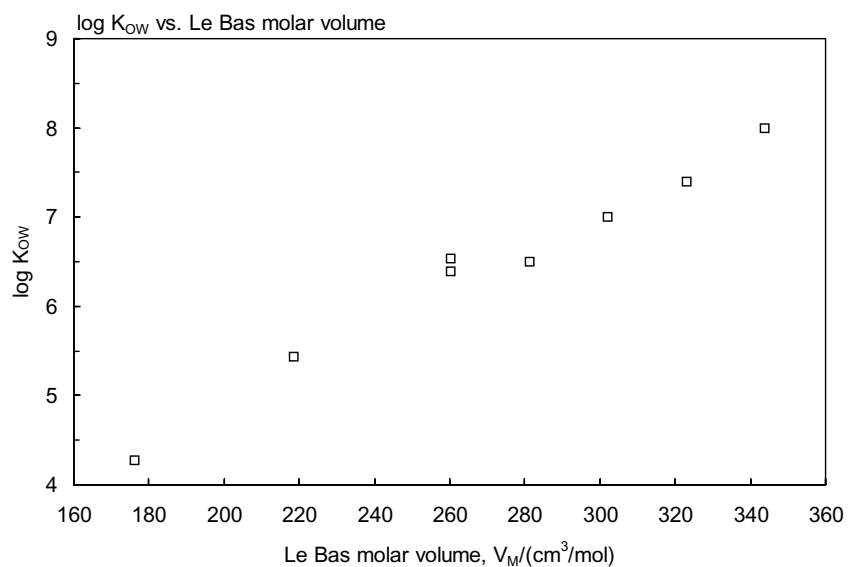


FIGURE 9.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated dibenzofurans.

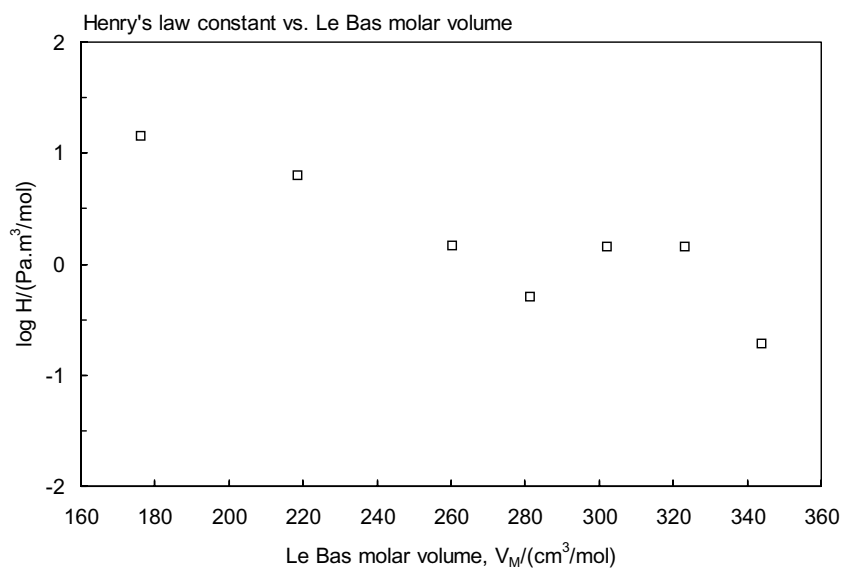


FIGURE 9.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated dibenzofurans.

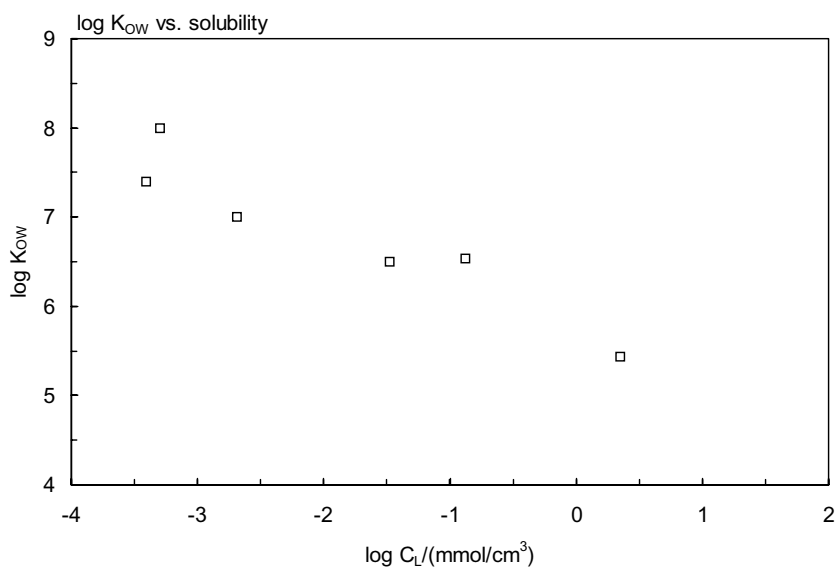


FIGURE 9.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated dibenzofurans.

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