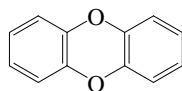

8 Chlorinated Dibenzo-*p*-dioxins

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8.1 LIST OF CHEMICALS AND DATA COMPILATIONS

8.1.1 DIBENZO-*p*-DIOXIN AND CHLORINATED DIBENZO-*p*-DIOXINS8.1.1.1 Dibenzo-*p*-dioxin

Common Name: Dibenzo-*p*-dioxin

Synonym: dibenzo-1,4-dioxin

Chemical Name: dibenzo-*p*-dioxin

CAS Registry No: 262-12-4

Molecular Formula: C₆H₄O₂C₆H₄

Molecular Weight: 184.191

Melting Point (°C):

120.5 (Lide 2003)

Boiling Point (°C):

266.0 (Rordorf 1986)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

143.82, 142.06 (calculated-liquid density, crystalline volume, Govers et al. 1990)

146.96 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

68.4 (Rordorf 1987)

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

92.250 (Rordorf 1987)

93.6 (Li et al. 2004)

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

23.2, 22.6 (obs., predicted, Rordorf 1986)

22.6 (Ruelle & Kesselring 1997)

23.2, 22.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

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

57 (Rordorf 1986, 1987, 1989)

58.63, 57.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.116 (mp at 120.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.842*, 0.90 (generator column-HPLC/UV, generator column-GC/ECD; Shiu et al. 1988)

0.90* (generator column-GC/ECD, measured range 4–25°C, Doucette & Andren 1988a)

0.90* (generator column-GC, measured range 4–40°C, Doucette & Andren 1988a)

S/(mol/L) = 8.85 × 10⁻⁷ exp(0.067·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a)

log x = -2541/(T/K) - 1.476; temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)

ln x = 4.1680 - 6087.88/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

7.16 (GC-RI correlation, Wang & Wong 2002)

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

0.055* (gas saturation-GC, Rordorf 1985ab, 1986, 1987, 1989)

0.050 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

0.512; 0.251 (supercooled liquid P_L, quoted exptl., calculated-SOFA Solubility-parameter-based-model, Govers & Krop 1998)

log (P/Pa) = 14.91018 - 4820.43/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.389; 0.251(GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

0.107* (30°C, Knudsen effusion method, measured range 30–60°C Li et al. 2002)

$\ln(P/\text{Pa}) = (34.944 \pm 0.444) - (11259 \pm 141)/(T/\text{K})$; temp range 303–333 K (Knudsen effusion technique, Li et al. 2002, 2004)

$\ln(P/\text{Pa}) = 34.319 - 11095/(T/\text{K})$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

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

12.40 (calculated-P/C, Shiu et al. 1987; 1988)

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

15.85; 10.96 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

4.31, 4.48, 4.38; 4.38, 4.46, 4.52 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)

4.26, 4.65 (Doucette 1985)

4.17, 4.46 (HPLC-RT correlation, Sarna et al. 1984)

4.26, 4.01; 4.34, 4.17 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)

4.20 (HPLC-RT correlation, Burkhard & Kuehl 1986)

4.37 (generator column-GC, Doucette & Andren 1987)

4.18 (HPLC-RT correlation, Doucette & Andren 1988b)

4.38 (recommended, Hansch et al. 1995)

4.15 (GC-RI correlation, Wang & Wong 2002)

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

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

4.49; 4.68 (lipid based BCF, guppy, quoted exptl., calculated-SOFA Solubility-parameter-base-model, Govers & Krop 1998)

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

4.34 (sediment/water, calculated-SOFA Solubility-parameter-base-model, Govers & Krop 1998)

4.01 (derived from soot-water distribution coeff., Bärning 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:

$k_{\text{OH}} = 4.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ corresponding to an atmospheric lifetime $\tau \sim 7 \text{ h}$ at room temp. (Atkinson 1987a)

$k_{\text{OH}}(\text{calc}) = 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987b)

$k_{\text{OH}} = 37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.4 \text{ d}$ based on the gas-phase reactions with OH radical and a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{\text{OH}} = 1.48 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime $\tau = 1.0 \text{ d}$, $k_{\text{NO}_3} = 3.9 \times 10^{-27} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetime $\tau = 4.9 \text{ d}$, and $k_{\text{O}_3} < 5 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau > 330 \text{ d}$ at $297 \pm 2 \text{ K}$ (Kwok et al. 1994)

$k_{\text{OH}}(\text{exptl}) = 14.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, corresponding to a tropospheric lifetime of 1.0 d (Kwok et al. 1995)

$k_{\text{OH}}^* = 12 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 345–385 K; and $k_{\text{OH}}(\text{calc}) = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime $\tau = 24 \text{ h}$ based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: room temp. gas-phase reaction rate constant $k = 4.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical corresponding to an atmospheric lifetime of about 7 h (Atkinson 1987a)

tropospheric lifetime $\tau = 0.4 \text{ d}$ calculated for dibenzo-*p*-dioxin based on the gas-phase reaction with OH radical (Atkinson 1991);

tropospheric lifetimes: $\tau(\text{calc}) = 1.0 \text{ d}$, 4.9 d and >330 d for reactions with OH radical, NO_3 radical and O_3 , respectively at room temp. (Kwok et al. 1994);

tropospheric lifetime $\tau(\text{calc}) = 1.0 \text{ d}$ with respect to reaction with the OH radical (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 8.1.1.1.1

Reported aqueous solubilities and vapor pressures of dibenzo-*p*-dioxin at various temperatures and the reported temperature dependence equations

Aqueous solubility				Vapor pressure			
Shiu et al. 1988		Doucette & Andren 1988		Rordorf 1987, 1989		Li et al. 2002	
generator column-HPLC/UV		generator column-GC/ECD		gas saturation		Knudsen effusion	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa
5	0.205	4.1	0.212	25	0.055	30	0.107
15	0.460	25	0.90	50	0.98	35	0.215
25	0.842	40	2.392	75	12.0	40	0.358
35	1.762			100	97	45	0.628
45	3.262	ΔH _{sol} /(kJ mol ⁻¹) = 48.6		125	630	50	1.14
		at 25 °C				55	1.90
ΔH _{sol} /(kJ mol ⁻¹) = 50.68				ΔH _v /(kJ mol ⁻¹) = 68.4		60	3.08
for 5–45 °C		S/(mol/L) = a·exp[b(t/°C)]		ΔH _{subl} /(kJ mol ⁻¹) = 92.25			
		a	8.85 × 10 ⁻⁷	ΔH _{fus} /(kJ mol ⁻¹) = 22.6		ln (P/Pa) = A – B/(T/K)	
		b	0.067	ΔS _{fus} /(J mol ⁻¹ K ⁻¹) = 57		A	34.994
		OR:				B	11259
		ln x = A – B/(T/K)					
		A	–1.476				
		B	2541				

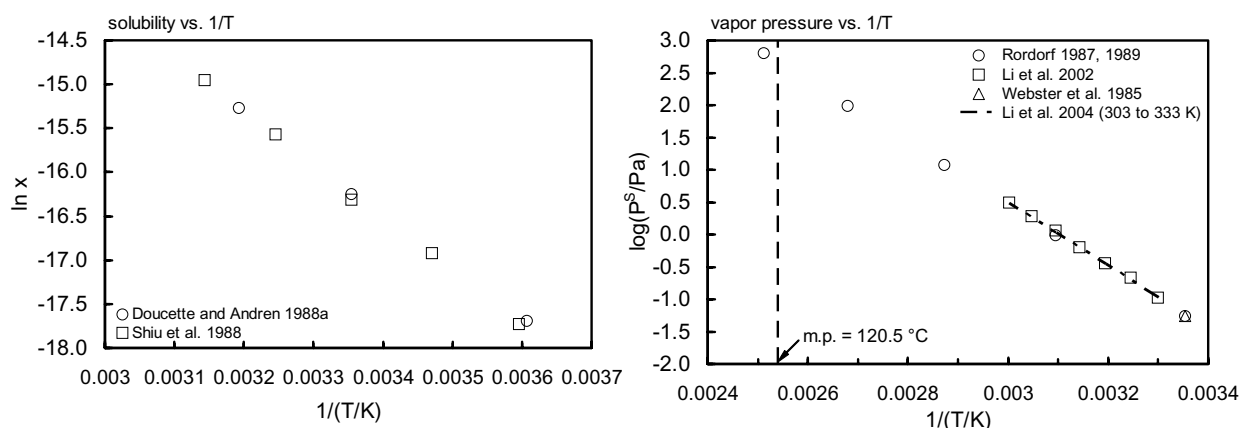
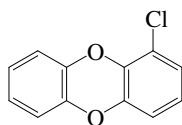


FIGURE 8.1.1.1.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for dibenzo-*p*-dioxin.

8.1.1.2 1-Chlorodibenzo-*p*-dioxin

Common Name: 1-Chlorodibenzo-*p*-dioxin

Synonym: 1-CDD, 1-MCDD

Chemical Name: 1-chlorodibenzo-*p*-dioxin

CAS Registry No: 39227-53-7

Molecular Formula: C₆H₄O₂C₆H₃Cl

Molecular Weight: 218.636

Melting Point (°C):

104.5–105.5 (Pohland & Yang 1972; quoted, Rordorf 1986,1987,1989)

Boiling Point (°C):

296.0 (Rordorf 1986)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

157.41, 158.07 (calculated-liquid density, crystalline volume, Govers et al. 1990)

156.19 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

76.2 (Rordorf 1987)

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

98.55 (Rordorf 1987)

100.5 (Li et al. 2004)

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

23.2, 21.4 (obs., predicted, Rordorf 1986)

23.2, 22.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

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

56.0 (Rordorf 1986,1987,1989)

61.34, 58.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.164 (mp at 105.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.417* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)

ln *x* = −0.68385 − 4912.15/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

1.51 (supercooled liquid S_L, GC-RI correlation; Wang & Wong 2002)

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

0.012* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989; quoted, Shiu et al. 1988)

log (P/Pa) = 15.35327 − 5150.4/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.0275 (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)

ln (P/Pa) = 35.353 − 11859/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

ln (P/Pa) = (36.087 ± 0.293) − (12085 ± 96)/(T/K); temp range 308–343 K (Knudsen effusion technique, Li et al. 2004)

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

8.38 (calculated-P/C, Shiu et al. 1988)

6.31; 4.57 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

7.76; 5.75 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

- 4.97, 5.20, 5.25; 5.05, 5.18, 5.23 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
4.91, 5.18 (HPLC-RT correlation, Sarna et al. 1984)
4.81, 4.52; 4.91, 5.74 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
4.75 (HPLC-RT correlation, Burkhard & Kuehl 1986)
5.05 (recommended, Hansch et al. 1995)
4.99 (GC-RI correlation; Wang & Wong 2002)

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

Additional data at other temperatures designated * are compiled at the end of this section:

- 7.86*; 8.34 (generator column-GC; calculated, Harner et al. 2000)
 $\log K_{OA} = -2.88 + 3200/(T/K)$; temp range 10–40°C (Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

- 5.17; 5.08 (lipid wt base, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

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

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

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

Volatilization:

Photolysis:

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:

$k_{OH}(\text{calc}) = 32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5 \text{ d}$ based on the gas-phase reactions with OH radical and a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{exptl}) = 4.7 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, corresponding to a tropospheric lifetime of 1.0 d (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5 \text{ d}$ calculated for a mono-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime for mono-chlorinated dioxin was 3.0 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 8.1.1.2.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1-chlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure		log K _{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K _{OA}
5	0.205	25	0.012	10	8.466
15	0.460	50	0.26	20	8.018
25	0.842	75	3.60	30	7.628
35	1.762	100	36.0	40	7.396
45	3.262	125	260	25	7.86
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 40.85$ for 5–45°C		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 76.2$ $\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 98.55$ $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 21.4$ $\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 56.0$		$\log K_{\text{OA}} = a + b/(T/\text{K})$ a -2.88 b 3200	
				enthalpy of phase change $\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 61.30$	

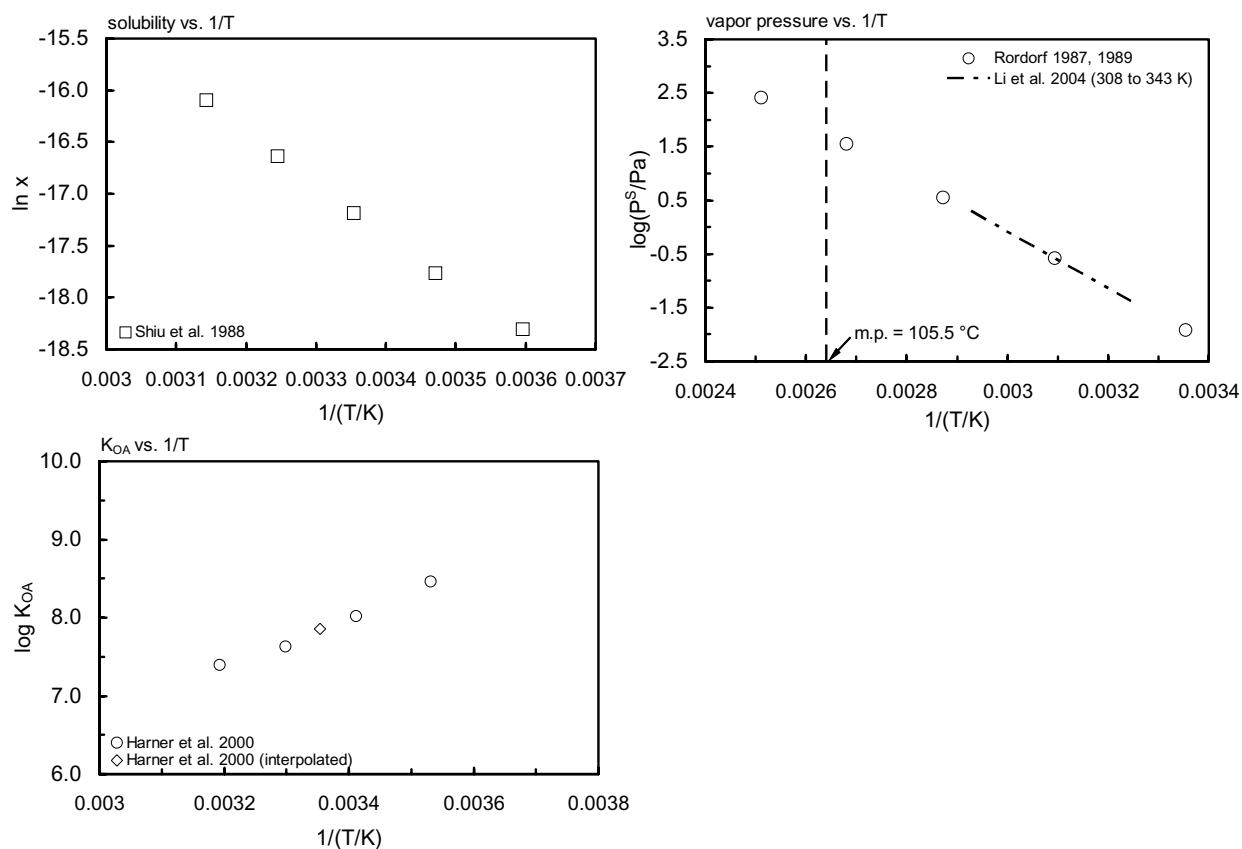
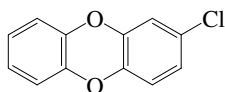


FIGURE 8.1.1.2.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1-chlorodibenzo-*p*-dioxin.

8.1.1.3 2-Chlorodibenzo-*p*-dioxin

Common Name: 2-Chlorodibenzo-*p*-dioxin

Synonym: 2-CDD, 2-MCDD

Chemical Name: 2-chlorodibenzo-*p*-dioxin

CAS Registry No: 39227-54-8

Molecular Formula: $C_{12}H_8ClO_2$

Molecular Weight: 218.636

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

88–89 (Pohland & Yang 1972)

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

298.0 (Rordorf 1986)

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

Molar Volume (cm^3/mol):

154.85, 155.15 (calculated-liquid density, crystalline volume, Govers et al. 1990)

153.09 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.2 (Rordorf 1987)

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

97.16 (Rordorf 1987)

98.1 (Li et al. 2004)

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

23.1, 18.5 (obs., predicted, Rordorf 1986)

18.5 (Ruelle & Kesselring 1997)

23.1, 21.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

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

51 (Rordorf 1987, 1989)

63.78, 57.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.236 (mp at $89^{\circ}C$)

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):

0.278*, 0.319 (generator column-HPLC/UV, generator column-GC/ECD, measured range $5-45^{\circ}C$, Shiu et al. 1988)

0.319* (generator column-GC/ECD, measured range $3.9-39^{\circ}C$, Doucette & Andren 1988a)

$S/(mol/L) = 4.88 \times 10^{-7} \exp(0.048 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range $4-40^{\circ}C$, Doucette & Andren 1988a); or

$\log x = -1777/(T/K) - 1.566$, temp range $4-40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

$\ln x = 4.093418 - 6448/(T/K)$; temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

1.44 (GC-RI correlation, 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):

0.017* (gas saturation-GC, Rordorf 1985a,b,1986,1987,1989)

0.016 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

$\log (P/Pa) = 15.2463 - 5071.88/(T/K)$; temp range $5-50^{\circ}C$ (regression eq. from literature data, Shiu & Ma 2000)

0.0262 (GC-RI correlation, Wang & Wong 2002)

$\ln(P/\text{Pa}) = 35.106 - 11679/(T/\text{K})$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (35.549 \pm 0.415) - (11794 \pm 134)/(T/\text{K})$, temp range 308–343 K (Knudsen effusion technique, Li et al. 2004)

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

14.82 (calculated-P/C, Shiu et al. 1988)
 12.60; 4.57 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 7.586; 4.57 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

5.36, 5.66, 5.71; 5.45, 5.64, 5.69 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 5.45, 5.64 (HPLC-RT correlation, Sarna et al. 1984)
 5.33, 5.00; 5.45, 5.29 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 5.08 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 4.94 (generator column-GC/ECD, Doucette & Andren 1987)
 4.98 (HPLC-RT correlation, Doucette & Andren 1988b)
 5.45 (recommended, Hansch et al. 1995)
 5.01 (GC-RI correlation, Wang & Wong 2002)

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

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

5.09 (guppy, Loonen et al. 1994)
 5.09; 5.12 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

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

3.92 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 5.35 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

Photolysis: photodegradation $t_{1/2} = 10$ min with simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988)
 photodegradation $k = 1.81 \text{ h}^{-1}$ with $t_{1/2} = 0.38$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

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

$k_{\text{OH}} = 32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5$ d for a mono-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{\text{OH}}(\text{exptl}) = 4.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 3.0$ d at room temp. (relative rate method, Kwok et al. 1995)

$k_{\text{OH}}(\text{calc}) = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Brubaker & Hites 1998)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5$ d calculated for a mono-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime for mono-chlorinated dioxin was 3.0 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

first-order photodegradation $k = 1.81 \text{ h}^{-1}$ with $t_{1/2} = 0.38$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: $t_{1/2} = 10$ min irradiated under simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 8.1.1.3.1

Reported aqueous solubilities and vapor pressures of 2-chlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure	
Shiu et al. 1988		Doucette & Andren 1988		Rordorf 1987, 1989	
generator column-HPLC/UV		generator column-GC/ECD		gas saturation-GC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
5	0.0603	3.9	0.133	25	0.017
15	0.137	25	0.319	50	0.36
25	0.278	39	0.7495	75	4.80
35	0.653			100	45.0
45	1.109			125	320

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 53.35$
5–45 $^{\circ}\text{C}$

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 34.0$
4–32 $^{\circ}\text{C}$

$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 78.1$
 $\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 97.16$
 $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.5$
 $\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 51$

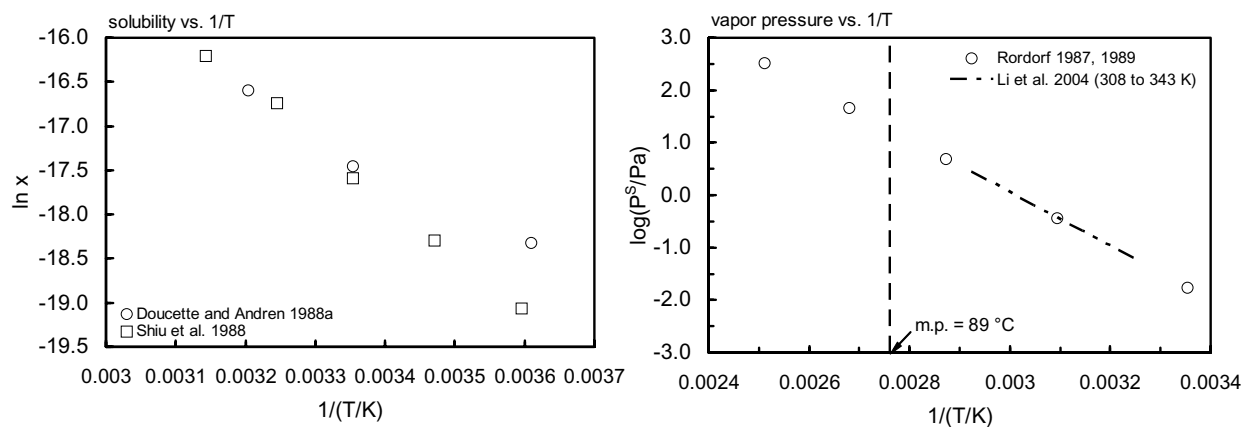
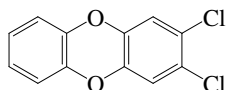


FIGURE 8.1.1.3.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2-chlorodibenzo-*p*-dioxin.

8.1.1.4 2,3-Dichlorodibenzo-*p*-dioxin

Common Name: 2,3-Dichlorodibenzo-*p*-dioxin

Synonym: 2,3-DCDD

Chemical Name: 2,3-dichlorodibenzo-*p*-dioxin

CAS Registry No: 29446-15-9

Molecular Formula: $C_{12}H_4O_2Cl_2$

Molecular Weight: 253.081

Melting Point (°C):

163–164 (Pohland & Yang 1972)

Boiling Point (°C):

358 (calculated, Rordorf 1986,1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

164.07 (calculated-liquid density, Govers et al. 1990)

162.67 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.8 (Rordorf 1987)

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

106.23 (Rordorf 1987)

106.2 (Li et al. 2004)

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

26.7 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

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

61 (Rordorf 1986,1987,1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.0433 (mp at 164°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0149* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)

$\ln x = 0.07859 - 6173.64/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

0.297 (GC-RI correlation, Wang & Wong 2002)

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

0.00039* (gas saturation-GC, Rordorf 1985a,b, 1986,1989)

0.0004 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

0.0020 (GC-RI correlation, Wang & Wong 2002)

$\log (P_L/\text{mmHg}) = 48.98 - 6446/(T/K) - 12.569 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln (P/\text{Pa}) = 35.096 - 12804/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln (P/\text{Pa}) = (35.081 \pm 0.374) - (12771 \pm 134)/(T/K)$; temp range 338–378 K (Knudsen effusion technique, Li et al. 2004)

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

6.61 (calculated-P/C, Shiu et al. 1988)

6.61; 2.51 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)

3.80; 2.51 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

- 4.70 (calculated, Kaiser 1983)
- 6.23, 5.60 (calculated-QSAR, quoted, Fiedler & Schramm 1990)
- 5.77 (calculated-SOFA model, Govers & Krop 1998)
- 5.738 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 5.80; 5.77 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

- 8.50 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 5.41 (lipid wt based, calculated-SOFA model, Govers & Krop 1998)

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

- 4.73 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
- 6.27 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

Photolysis:

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

$k_{OH}(\text{calc}) = 22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (22 - 28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5\text{--}0.7$ d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (5.9 - 7.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.0\text{--}2.4$ d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

$k_{OH}(\text{calc}) = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Brubaker & Hites 1998)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_2 = 0.092 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5\text{--}0.7$ d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime $\tau = 2.0\text{--}2.4$ d for the reaction with OH radical (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

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

biological $t_{1/2} = 7$ d in rainbow trout (Niimi & Oliver 1986);

biological $t_{1/2} = 2\text{--}7$ d in trout (Niimi 1987).

TABLE 8.1.1.4.1
Reported aqueous solubilities and vapor pressures of 2,3-dichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure	
Shiu et al. 1988		Rordorf 1987, 1989	
generator column-HPLC/UV		gas saturation-GC	
t/°C	S/g·m ⁻³	t/°C	P/Pa
5	0.00368	25	0.00039
15	0.00716	50	0.0011
25	0.0149	75	0.18
35	0.0304	100	2.20
45	0.0586	125	19.0

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 51.3$
5–45 °C

$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 77.8$
 $\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 106.23$
 $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 26.7$
 $\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 61$

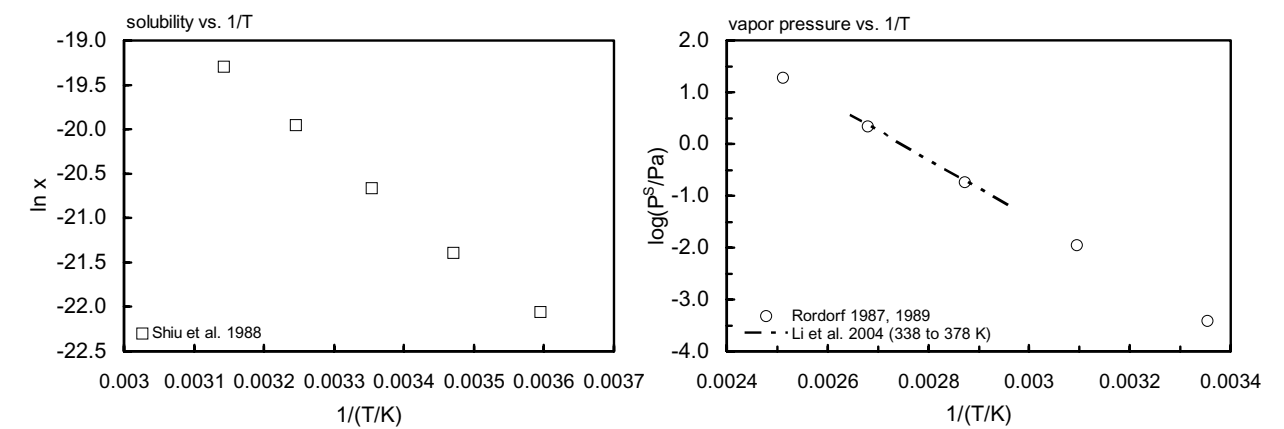
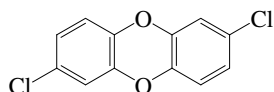


FIGURE 8.1.1.4.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,3-dichlorodibenzo-*p*-dioxin.

8.1.1.5 2,7-Dichlorodibenzo-*p*-dioxin

Common Name: 2,7-Dichlorodibenzo-*p*-dioxin

Synonym: 2,7-DCDD

Chemical Name: 2,7-dichlorodibenzo-*p*-dioxin

CAS Registry No: 33857-26-0

Molecular Formula: $\text{ClC}_6\text{H}_3\text{O}_2\text{C}_6\text{H}_3\text{Cl}$

Molecular Weight: 253.081

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

210 (Lide 2003)

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

374.5 (calculated, Rordorf 1987, 1989)

Density (g/cm^3):

1.647 (calculated, Boer et al. 1972)

Molar Volume (cm^3/mol):

165.88, 162.89 (calculated-liquid density, crystalline volume, Govers et al. 1990)

162.87 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

76.4 (Rordorf 1987)

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

105.51 (Rordorf 1987)

113.8 (Li et al. 2004)

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

26.8 (Rordorf 1986, 1987; Ruelle & Kesselring 1997)

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

55 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.0188 (mp at 201°C)

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

0.00375* (generator column-HPLC/UV, Shiu et al. 1988)

0.00224 (generator column-GC/MS, Santl et al. 1994)

$\ln x = -3.48833 - 5543.9/(T/\text{K})$; temp range 5 – 50°C (regression eq. of literature data, Shiu & Ma 2000)

0.311 (GC-RI correlation, Wang & Wong 2002)

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

0.00012* (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989; quoted, Shiu et al. 1988)

0.00013 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

$\log (P/\text{Pa}) = 14.60827 - 5523.34/(T/\text{K})$ temp range 5 – 50°C (regression eq. from literature data, Shiu & Ma 2000)

0.00219 (GC-RI correlation, Wang & Wong 2002)

$\log (P_L/\text{mmHg}) = 49.61 - 6624/(T/\text{K}) - 12.569 \cdot \log (T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln (P/\text{Pa}) = 33.637 - 12718/(T/\text{K})$; temp range 298 – 398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln (P/\text{Pa}) = (36.293 \pm 0.648) - (13686 \pm 245)/(T/\text{K})$; temp range 358 – 393 K (Knudsen effusion technique, Li et al. 2004)

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

- 8.11 (calculated-P/C, Shiu et al. 1988)
- 6.98 (gas stripping-GC/MS, Santl et al. 1994)
- 8.13; 2.82 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 3.89; 2.82 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

- 6.28, 6.64, 6.72; 6.38, 6.62, 6.71 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 6.62, 6.39 (HPLC-RT correlation, Sarna et al. 1984)
- 6.27, 5.86; 6.39, 6.17 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 5.75 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 6.38 (recommended, Sangster 1993)
- 6.38 (recommended, Hansch et al. 1995)
- 5.77 (GC-RI correlation, Wang & Wong 2002)

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

Additional data at other temperatures designated * are compiled at the end of this section:

- 8.36*; 8.67 (generator column-GC; calculated, Harner et al. 2000)
- log $K_{OA} = -3.74 + 3610/(T/K)$; temp range 10–40°C (Harner et al. 2000)
- 8.48 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 1.7, 2.9 (guppy, in whole fish, in lipid, Gobas et al. 1987)
- 2.56, 3.68 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
- 5.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{oc} :

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

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

Volatilization:

Photolysis: photodegradation $t_{1/2} = 46$ min in an aqueous solution assisted by TiO₂ at 2.0 g/L under simulated sunlight (Barbeni et al. 1986)

photodegradation $t_{1/2} = 1$ h with irradiation under simulated sunlight in aerated aqueous suspension of semiconductor TiO₂ at 4.0 g/L and pH 3 (Pelizzetti et al. 1988)

photolysis $k = 8.9 \times 10^{-2} \text{ min}^{-1}$ with $t_{1/2} = 7.8$ min in pure water, and rate constant $k = 0.16 \text{ min}^{-1}$ with $t_{1/2} = 4.3$ min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000).

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

$k_{OH}(\text{calc}) = (26\text{--}28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (22\text{--}28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5\text{--}0.7$ d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (5.9\text{--}7.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.0\text{--}2.4$ d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

$k_{OH}(\text{calc}) = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Brubaker & Hites 1998)

$k_{OH}^* = 23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured temp range 355–395 K, and $k_{OH}(\text{calc}) = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, with a calculation lifetime $\tau = 65$ h based on gas-phase OH reactions (Brubaker & Hites 1998)

Biodegradation:

Biotransformation: metabolic elimination $k_m = 0.23 \text{ d}^{-1}$ (goldfish, 20°C, 96-h exposure, Sijm & Opperhuizen 1988)

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

$k_2 = 0.462 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

$k_1 = 390 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.23 \text{ d}^{-1}$ (goldfish, 20°C, 96-h exposure, Sijm & Opperhuizen 1988)

$k_1 = 543 \text{ d}^{-1}$; $k_2 = 1.5 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5\text{--}0.7$ d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric calculated lifetime $\tau = 2.0\text{--}2.4$ d for the reaction with OH radical (Kwok et al. 1995);

calculated lifetime $\tau = 65$ h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: photodegradation $t_{1/2} = 1$ h with irradiation under simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988);

photolysis rate constant $k = 8.9 \times 10^{-2} \text{ min}^{-1}$ with $t_{1/2} = 7.8$ min in pure water, and $k = 1.6 \times 10^{-1} \text{ min}^{-1}$ with $t_{1/2} = 4.3$ min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000).

Groundwater:

Sediment:

Soil:

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

biological $t_{1/2} = 2$ d in rainbow trout (Niimi & Oliver 1986);

biological $t_{1/2} = 2\text{--}7$ d in trout (Niimi 1987).

TABLE 8.1.1.5.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,7-dichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	log K_{OA}
5	0.00109	25	0.0001	10	9.020
15	0.00201	50	0.0033	20	8.564
25	0.00375	75	0.056	30	8.106
35	0.00727	100	0.64	40	7.818
45	0.0134	125	5.4	25	7.36
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 50.68$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 76.4$		$\log K_{OA} = a + b/(T/K)$	
25 $^{\circ}\text{C}$		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 105.51$		a	-3.74
		$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 26.8$		b	3610
		$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 55$		enthalpy of phase change	
				$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 69.0$	

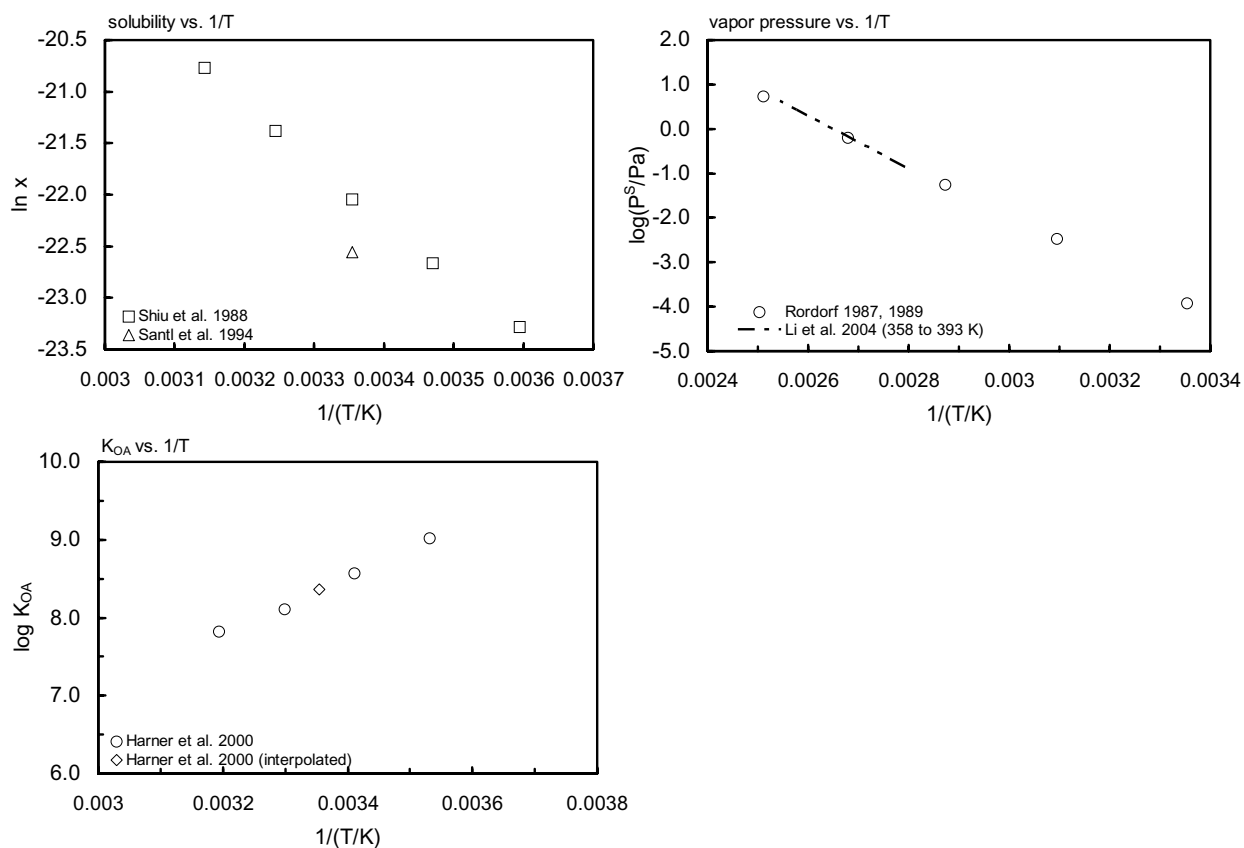
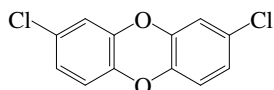


FIGURE 8.1.1.5.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,7-dichlorodibenzo-*p*-dioxin.

8.1.1.6 2,8-Dichlorodibenzo-*p*-dioxin

Common Name: 2,8-Dichlorodibenzo-*p*-dioxin

Synonym: 2,8-TCDD

Chemical Name: 2,8-dichlorodibenzo-*p*-dioxin

CAS Registry No: 38964-22-6

Molecular Formula: $\text{ClC}_6\text{H}_3\text{O}_2\text{C}_6\text{H}_3\text{Cl}$

Molecular Weight: 253.081

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

150.5–151 (Pohland & Yang 1972; Rordorf 1986,1987,1989)

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

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

165.88, 167.2 (calculated-liquid density, crystalline volume, Govers et al. 1990)

160.63 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.1 (Rordorf 1987)

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

109.01 (Rordorf 1987)

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

23.2 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

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

55 (Rordorf 1986,1987,1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F : 0.058 (mp at 151°C)

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

0.0167* (generator column-GC/ECD, measured range $5\text{--}45^{\circ}\text{C}$, Shiu et al. 1988)

$\ln x = -2.54177 - 5379/(T/\text{K})$; temp range $5\text{--}50^{\circ}\text{C}$ (regression eq. of literature data, Shiu & Ma 2000)

0.311 (supercooled liquid S_L , GC-RI correlation, Wang & Wong 2002)

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

0.00014* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989)

0.00013 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

$\log (P/\text{Pa}) = 15.25386 - 5699.96/(T/\text{K})$; temp range $5\text{--}50^{\circ}\text{C}$ (regression eq. from literature data, Shiu & Ma 2000)

0.00219 (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

0.00150 (solid P_S , gas saturation-GC/MS, Mader & Pankow 2003)

0.0260 (supercooled liquid P_L , calculated from P_S assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, Mader & Pankow 2003)

$\log (P_L/\text{mmHg}) = 49.89 - 6705/(T/\text{K}) - 12.569 \cdot \log (T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

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

2.13 (calculated- P/C , Shiu et al. 1988)

2.14; 2.29 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)

3.89; 2.29 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

- 4.70 (calculated, Kaiser 1983)
- 5.60 (selected, Shiu et al. 1988)
- 5.68 (calculated-SOFA model, Govers & Krop 1998)
- 5.638 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 5.77; 5.68 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
- 5.34, 5.50, 5.75, 5.58 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

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

Additional data at other temperatures designated * are compiled at the end of this section:

- 8.36*; 8.65 (generator column-GC; measured range 10–40°C; calculated, Harner et al. 2000)
- log $K_{OA} = -3.74 + 3610/(T/K)$; temp range 10–40°C, (Harner et al. 2000)
- 8.48 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 2.77, 2.82 (goldfish: treated with metabolic inhibitor PBO, untreated, Sijm & Opperhuizen 1988)
- 5.42 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} :

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

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

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:

$k_{OH}(\text{calc}) = (26-28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (22-28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5-0.7 \text{ d}$ for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (5.9-7.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.0-2.4 \text{ d}$ for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation: metabolic elimination rate constant from goldfish was estimated to be 0.35 d^{-1} (Sijm & Opperhuizen 1988).

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

$k_1 = 390 \text{ L kg}^{-1} \cdot \text{d}^{-1}$; $k_2 = 0.23 \text{ d}^{-1}$ (goldfish, Opperhuizen & Sijm 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5 - 0.7 \text{ d}$ calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime $\tau = 2.0 - 2.4 \text{ d}$ for the reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

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

biological $t_{1/2} = 2-7 \text{ d}$ in trout (Niimi 1987).

TABLE 8.1.1.6.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,8-dichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure		log K _{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m ⁻³			t/°C	log K _{OA}
5	0.00422	25	0.0001	10	9.020
15	0.00859	50	0.0042	20	8.564
25	0.0167	75	0.078	30	8.106
35	0.0275	100	0.97	40	7.818
45	0.0515	125	8.80	25	8.36
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 50.04$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 84.1$		$\log K_{\text{OA}} = a + b/(T/\text{K})$	
5–45 °C		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 109.01$		a	
		$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 23.3$		b	
		$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 55$		enthalpy of phase change	
				$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 69.0$	

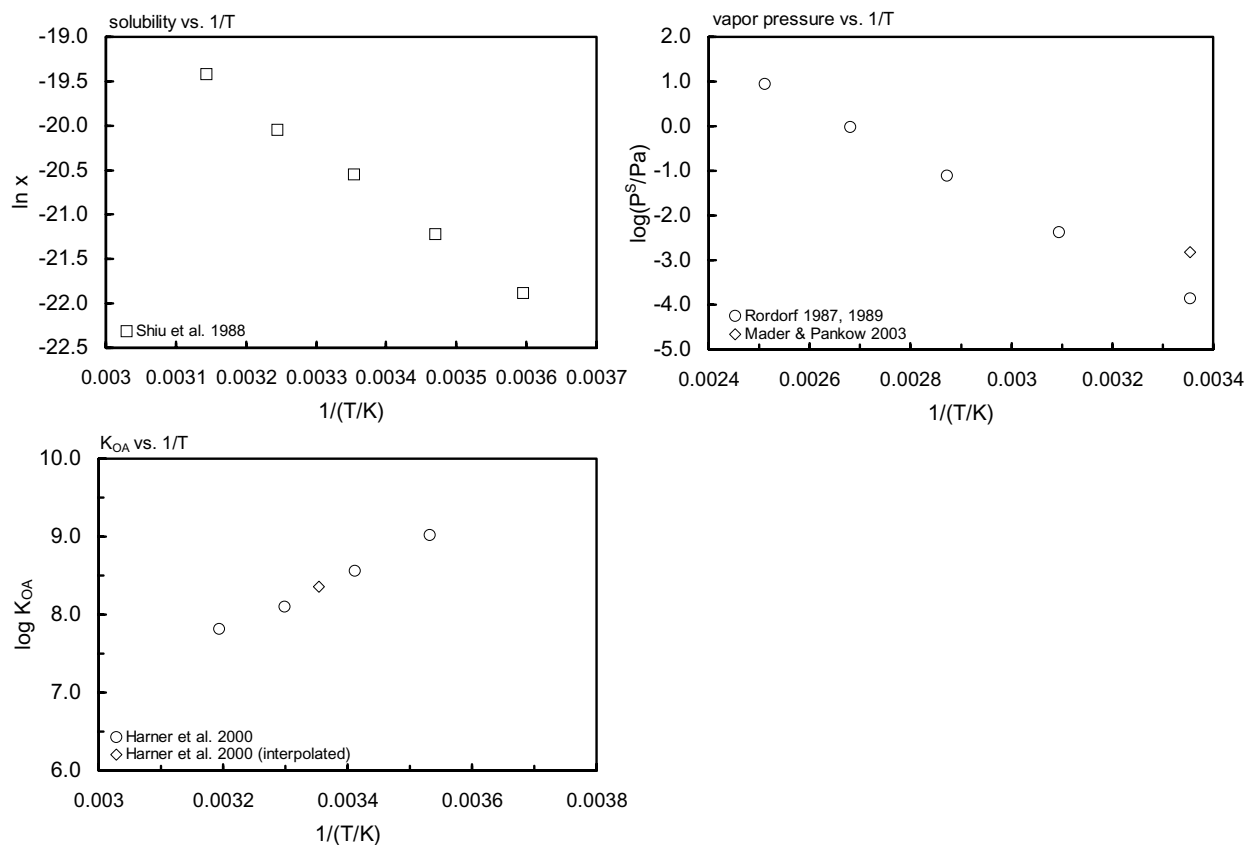
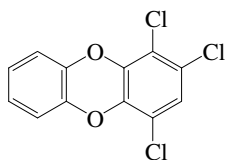


FIGURE 8.1.1.6.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,8-dichlorodibenzo-*p*-dioxin.

8.1.1.7 1,2,4-Trichlorodibenzo-*p*-dioxin

Common Name: 1,2,4-Trichlorodibenzo-*p*-dioxin

Synonym: 1,2,4-TCDD

Chemical Name: 1,2,4-trichlorodibenzo-*p*-dioxin

CAS Registry No: 39227-58-2

Molecular Formula: $C_{12}H_5Cl_3O_2$, $C_6H_4O_2C_6HCl_3$

Molecular Weight: 287.526

Melting Point (°C):

128–129 (Pohland & Yang 1972; quoted, Rordorf 1986, 1987, 1989)

Boiling Point (°C):

375.0 (calculated, Rordorf 1986, 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

179.66 (calculated-liquid density, Govers et al. 1990)

173.60 (liquid molar volume, Govers et al. 1995)

239.7 (calculated-Le Bas method at normal boiling)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.9 (Rordorf 1987)

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

118.79 (Rordorf 1987)

121.0 (Li et al. 2004)

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

33.9 (Rordorf 1986, 1987)

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

67 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.0954 (mp at 129°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00841* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)

0.00695 (generator column-GC/MS, Santl et al. 1994)

$\ln x = -2.4909 - 5626.95/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

0.091 (supercooled liquid S_L , GC-RI correlation, Wang & Wong 2002)

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

0.0001* (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)

0.0001 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

$\log(P/\text{Pa}) = 16.9148 - 6235.45/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.000324 (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

5.07×10^{-4} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

5.43×10^{-3} (supercooled liquid P_L , calculated from measured P_s assuming $\Delta S_{\text{fus}} = 56$ J/mol K, Mader & Pankow 2003)

$\log(P_L/\text{mmHg}) = 47.18 - 6479/(T/K) - 12.028 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/\text{Pa}) = 38.948 - 14358/(T/\text{K})$; temp range 298 – 398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (39.303 \pm 0.605) - (14550 \pm 221)/(T/\text{K})$; 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):

- 3.84 (calculated-P/C, Shiu et al. 1988)
- 3.64 (gas stripping-GC/MS, Santl et al. 1994)
- 3.72; 1.82 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 2.29; 1.82 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

- 7.40, 7.77, 7.69; 7.47, 7.76, 7.68 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 7.45, 7.76 (HPLC-RT correlation, Sarna et al. 1984)
- 7.36, 6.86; 7.45, 7.11 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 6.45 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 7.47 (recommended, Hansch et al. 1995)
- 6.34 (GC-RI correlation, Wang & Wong 2002)

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

- 8.97 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 1.90, 3.10 (guppy, in whole fish, in lipid, Gobas et al. 1987)
- 2.82, 3.95 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
- 5.42 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

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

- 7.01 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 5.87 (derived from soot-water distribution coeff., Bärning 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 (oxidative degradation rate of water dissolved PCDD by ozone) is $1.27 \times 10^6 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{OH}(\text{calc}) = (21\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (17\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (4.5\text{--}5.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.5\text{--}3.3 \text{ d}$ for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

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

- $k_2 = 0.058 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)
- $k_1 = 601 \text{ d}^{-1}$; $k_2 = 0.91 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radical (Atkinson 1991); the calculated tropospheric lifetime $\tau = 2.5\text{--}3.3 \text{ d}$ for the gas phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone $k = 1.27 \times 10^6 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987).

Sediment:

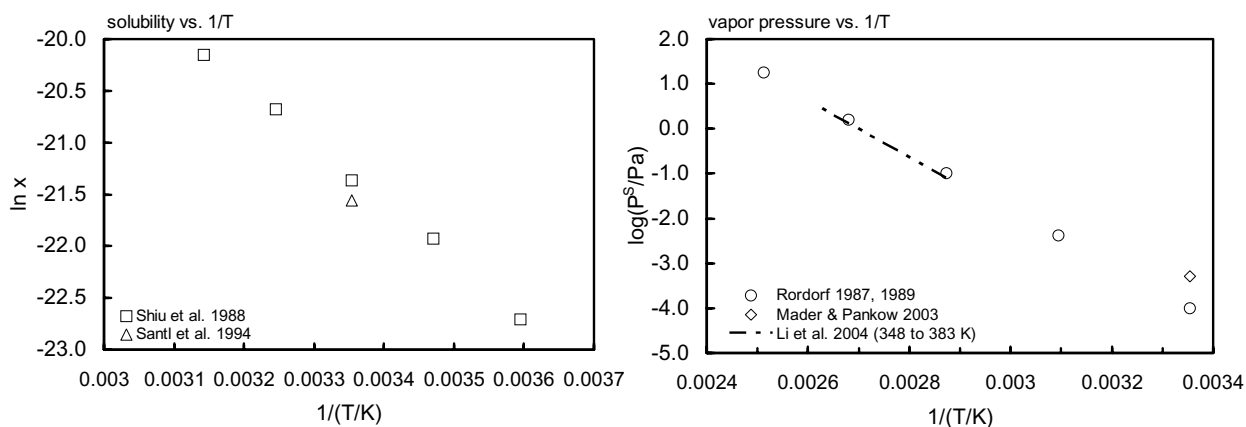
Soil:

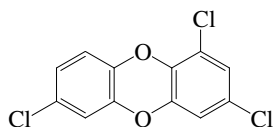
Biota: mean biological $t_{1/2} \sim 10$ d in rainbow trout (Niimi 1986); $t_{1/2} = 12$ d in rainbow trout (Niimi & Oliver 1986);biological $t_{1/2} = 12$ d in trout (Niimi 1987)**TABLE 8.1.1.7.1****Reported aqueous solubilities and vapor pressures of 1,2,4-trichlorodibenzo-*p*-dioxin at various temperatures**

Aqueous solubility		Vapor pressure	
Shiu et al. 1988		Rordorf 1987, 1989	
generator column-HPLC/UV		gas saturation-GC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
5	0.00219	25	0.0001
15	0.00477	50	0.0042
25	0.00841	75	0.1
35	0.0167	100	1.6
45	0.0282	125	18

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 46.62$
 $5\text{--}45^{\circ}\text{C}$

$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 83.9$
 $\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 118.79$
 $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 33.9$
 $\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 84$

**FIGURE 8.1.1.7.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,4-trichlorodibenzo-*p*-dioxin.

8.1.1.8 1,3,7-Trichlorodibenzo-*p*-dioxin

Common Name: 1,3,7-Trichlorodibenzo-*p*-dioxin

Synonym: 1,3,7-TCDD

Chemical Name: 1,3,7-trichlorodibenzo-*p*-dioxin

CAS Registry No: 67026-17-5

Molecular Formula: $C_{12}H_5Cl_3O_2$, $ClC_6H_3O_2C_6H_2Cl_2$

Molecular Weight: 287.526

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

148.5 (Rordorf 1986, 1987, 1989)

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

398 (calculated, Rordorf 1986, 1987, 1989)

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

Molar Volume (cm^3/mol):

170.18 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.4 (Rordorf 1987)

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

116.2 (Rordorf 1987)

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

28.4 (Rordorf 1986, 1987)

30.8, 25.7 (reported exptl., calculated, Chickos et al. 1999)

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

67 (Rordorf 1986, 1987, 1989)

73.04, 61.0 (reported exptl., calculated, Chickos 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S = 56$ J/mol K), F: 0.0614 (mp at $148.5^{\circ}C$)

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

0.0974 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0997; 0.0974 (supercooled liquid S_L , GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

3.60×10^{-5} * (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)

3.63×10^{-4} (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

$\log(P_L/mmHg) = 48.01 - 6714/(T/K) - 12.028 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

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

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

2.34, 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

6.31; 6.19 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

Bioconcentration Factor, log BCF:

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

Sorption Partition Coefficient, log K_{OC} :

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

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

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 (oxidative degradation rate of water dissolved PCDD by ozone) is $1.27 \times 10^6 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987)

$k_{OH}(\text{calc}) = (21\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (17\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (4.5\text{--}5.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.5\text{--}3.3 \text{ d}$ for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); the calculated tropospheric lifetime $\tau = .5\text{--}3.3 \text{ d}$ for the gas phase reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone $k = 1.27 \times 10^6 \text{ L} \cdot \text{g}^{-1} \cdot \text{min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987).

Sediment:

Soil:

Biota:

TABLE 8.1.1.8.1

Reported vapor pressures of 1,3,7-trichlorodibenzo-*p*-dioxin at various temperatures

Rordorf 1987, 1989	
gas saturation-GC/ECD	
$t/^\circ\text{C}$	P/Pa
25	3.6×10^{-5}
50	1.4×10^{-3}
75	3.1×10^{-2}
100	0.45
125	4.70
$\Delta H_v/(\text{kJ mol}^{-1}) = 86.4$	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 116.2$	
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 28.4$	

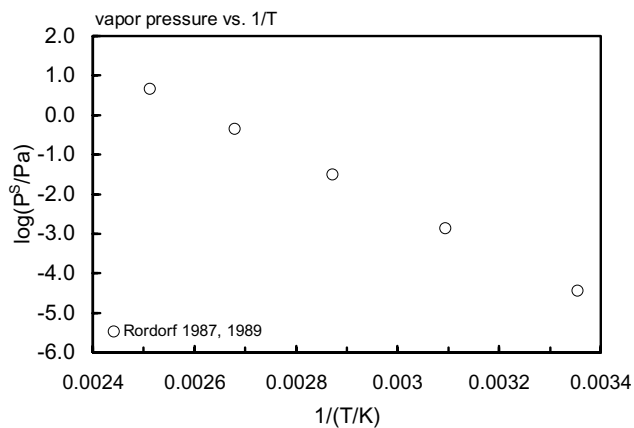
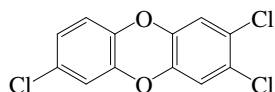


FIGURE 8.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3,7-trichlorodibenzo-*p*-dioxin.

8.1.1.9 2,3,7-Trichlorodibenzo-*p*-dioxin

Common Name: 2,3,7-Trichlorodibenzo-*p*-dioxin

Synonym: 2,3,7-TCDD

Chemical Name: 2,3,7-trichlorodibenzo-*p*-dioxin

CAS Registry No: 33857-28-2

Molecular Formula: $C_{12}H_5Cl_3O_2$, $ClC_6H_3O_2C_6H_2Cl_2$

Molecular Weight: 287.526

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

162–163 (Rordorf 1986, 1987, 1989)

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

408.4 (calculated, Rordorf 1986, 1987, 1989)

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

Molar Volume (cm^3/mol):

179.11 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.2 (Rordorf 1987)

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

119.759 (Rordorf 1987)

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

30.9 (Rordorf 1986, 1987)

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

71 (Rordorf 1986, 1987, 1989)

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

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

0.0548 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0674; 0.0548 (supercooled liquid S_L , GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

0.000012* (calculated, Rordorf 1985a,b, 1986, 1987, 1989)

2.14×10^{-4} (supercooled liquid P_L , GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\log(P_L/mmHg) = 48.21 - 6829/(T/K) - 12.028 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

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

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

2.04; 1.78 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

6.46; 6.33 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

6.47 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

9.14*, 9.28 (generator column-GC/ECD, measured range $0-40^{\circ}C$, calculated, Harner et al. 2000)

$\log K_{OA} = -5.35 + 4320/(T/K)$ (generator column-GC/ECD, measured range $0-40^{\circ}C$, Harner et al. 2000)

9.42 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

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

Sorption Partition Coefficient, log K_{OC} :

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

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

Volatilization:

Photolysis: photolysis rate $k = 2.03 \times 10^{-4} \text{ s}^{-1}$ at 313 nm using a Hanovia 450-W mercury lamp in hexane solution (Dulin et al. 1986)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{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 of water dissolved PCDD by ozone) is $1.27 \times 10^6 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987)

$k_{OH}(\text{calc}) = (21\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (17\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (4.5\text{--}5.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.5\text{--}3.3 \text{ d}$ for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric lifetime $\tau(\text{calc}) = 2.5\text{--}3.3 \text{ d}$ for the gas phase reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone $k = 1.27 \times 10^6 \text{ L g}^{-1} \cdot \text{min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987).

Sediment:

Soil:

Biota:

TABLE 8.1.1.9.1

Reported vapor pressures and octanol-air partition coefficients of 2,3,7-trichlorodibenzo-*p*-dioxin at various temperatures

Vapor pressure		log K_{OA}	
Rordorf 1987, 1989		Harner et al. 2000	
vapor pressure correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	K_{OA}
25	1.2×10^{-5}	0	10.573
50	5.2×10^{-4}	10	9.816
75	1.3×10^{-2}	20	9.313
100	0.21	30	8.935
125	2.3	40	8.497
		25	9.28
$\Delta H_v/(\text{kJ mol}^{-1}) = 87.2$		$\log K_{OA} = a + b/(T/K)$	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 119.76$		a	-5.35
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 30.9$		b	4320
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 82.7$	

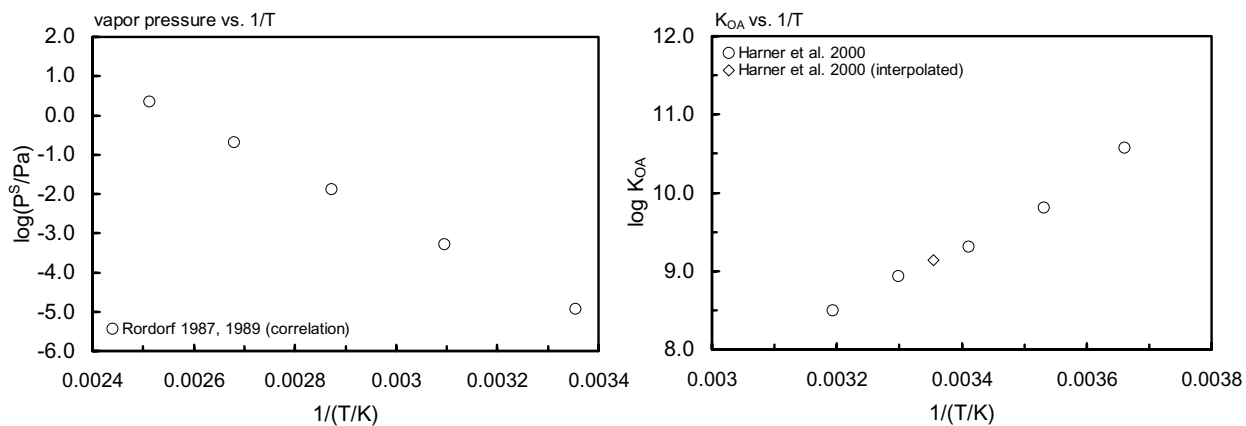
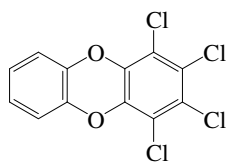


FIGURE 8.1.1.9.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 2,3,7-trichlorodibenzo-*p*-dioxin.

8.1.1.10 1,2,3,4-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4-TCDD

Chemical Name: 1,2,3,4-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 30746-58-8

Molecular Formula: C₁₂H₄O₂Cl₄

Molecular Weight: 321.971

Melting Point (°C):

189 (Pohland & Yang 1972; Rordorf 1986,1987,1989)

Boiling Point (°C):

419 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

186.71 (calculated-liquid density, Govers et al. 1990)

186.10 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.6 (Rordorf 1987)

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

118.53 (Rordorf 1987)

111.3 (Li et al. 2004)

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

31.2 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

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

68 (Rordorf 1986,1987,1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0246 (mp at 189°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00063*, 0.00047 (generator column-HPLC/UV, generator column-GC/ECD, Shiu et al. 1988)

0.00047* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988a)

S/(mol/L) = 2.75 × 10⁻¹⁰ exp(0.065·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or

log x = -2447/(T/K) - 2.373, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)

0.000388 (generator column-GC/MS, Santl et al. 1994)

ln x = -10.5076 - 3984/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

0.0165 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

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

0.0000064* (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)

1.00 × 10⁻⁵ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

1.04 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)

6.30 × 10⁻⁶ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

6.37 × 10⁻⁴ (corrected supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1998)

2.48 × 10⁻⁶ (solid vapor pressure calculated from reported P_L, Delle Site 1997)

log (P/Pa) = 15.59851 - 6199.79/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

2.75 × 10⁻⁵ (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)

2.26×10^{-5} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

9.66×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56$ J/mol K, Mader & Pankow 2003)

$\log (P_L/\text{mmHg}) = 45.97 - 6777/(T/K) - 11.499 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln (P/\text{Pa}) = 35.917 - 14276/(T/K)$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln (P/\text{Pa}) = (33.217 \pm 0.442) - (13386 \pm 173)/(T/K)$; temp range 378–403 K (Knudsen effusion technique, Li et al. 2004)

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

3.77 (calculated-P/C, Shiu et al. 1988)

2.02 (gas stripping-GC/MS, Santl et al. 1994)

3.02; 1.35 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)

1.15; 1.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

8.65, 8.90, 8.96; 8.66, 8.91, 8.97 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)

8.64, 8.91 (HPLC-RT correlation, Sarna et al. 1984)

8.63, 8.02; 8.64, 8.07 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)

7.18, 7.08 (HPLC-RT correlation, Burkhard & Kuehl 1986)

6.20 (generator column-GC/ECD, Doucette & Andren 1987)

6.85 (HPLC-RT correlation, Doucette & Andren 1988b)

6.48 (shake flask/slow stirring method-GC/ECD, mixture from fly-ash extract, Sijm et al. 1989a)

7.18 (recommended, Sangster 1993)

7.18 (recommended, Hansch et al. 1995)

7.04 (GC-RI correlation, Wang & Wong 2002)

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

Additional data at other temperatures designated * are compiled at the end of this section:

9.410 (calculated- K_{ow}/K_{aw} , Paterson et al. 1991)

9.70*; 9.86 (generator column-GC; calculated, Harner et al. 2000)

$\log K_{OA} = -4.96 + 4370/(T/K)$; temp range 10–40°C (Harner et al. 2000)

9.64 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

2.20, 3.40 (guppy, in whole fish, in lipid, Gobas et al. 1987)

2.90, 4.02 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)

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

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

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

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

Photolysis: solution photolysis $t_{1/2} = 1294$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 560$ min on a clean glass surface under the same conditions (Nestrick et al. 1980)

sunlight induced photolysis $t_{1/2} = 380$ min in isooctane solution and sunlight induced solid phase $t_{1/2} = 65$ h of TCDD dispersed as solid films (Buser 1988);

photodegradation $t_{1/2} = 88$ h for 1,2,3,4-TCDD adsorbed to clean silica gels in a rotary photo-reactor by filtered <290 nm of light (Koester & Hites 1992);

first-order photodegradation $k = 0.98$ h⁻¹ with $t_{1/2} = 0.71$ h when loaded on TiO₂ film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000)

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

k (oxidative degradation rate of water dissolved PCDD by ozone) is 4.73×10^5 L g⁻¹ min⁻¹ under alkaline condition at pH 10 and 20°C (Palaschek & Scholz 1987)

$k_{OH}(\text{calc}) = (16 - 19) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0 \text{ d}$ based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ at room temp. (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.0 - 5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2 \text{ d}$ for a tri-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

$k_{\text{OH}}^* = 8.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 306 – 366 K (Brubaker & Hites 1997)

$k_{\text{OH}}(\text{calc}) = 8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Brubaker & Hites 1998)

Biodegradation:

Biotransformation:

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

$k_2 = 0.016 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986)

$k_1 = 953 \text{ d}^{-1}$; $k_2 = 1.20 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

$k_1 = 35 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 > 0.23 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, $104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.802.0 \text{ d}$ calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime $\tau = 2.8\text{--}7.2 \text{ d}$ for the gas phase reaction with OH radical (Kwok et al. 1995);

first-order photodegradation $k = 0.98 \text{ h}^{-1}$ with $t_{1/2} = 0.71 \text{ h}$ when loaded on TiO_2 film under UV ($\lambda > 300 \text{ nm}$) or solar light irradiation in the air (Choi et al. 2000).

Surface water: sunlight induced photolysis $t_{1/2} = 380 \text{ min}$ in isooctane min and $t_{1/2} = 65 \text{ h}$ dispersed as solid films (Buser 1988).

Groundwater:

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

Soil: degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ (estimated, Suzuki et al. 2000).

Biota: mean $t_{1/2} \sim 43 \text{ d}$ in rainbow trout (Niimi 1986);

biological $t_{1/2} = 43 \text{ d}$ in rainbow trout (Niimi & Oliver 1986);

biological $t_{1/2} = 5\text{--}14 \text{ d}$ in trout (Niimi 1987);

$t_{1/2} < 0.3 \text{ d}$ for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993)

TABLE 8.1.1.10.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4-tetrachlorodibenzo-p-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Shiu et al. 1988		Doucette & Andren 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		generator column-GC/ECD		gas saturation-GC/ECD		generator column-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K_{OA}
5	0.00034	4	0.00011	25	6.4×10^{-6}	0	11.131
15	0.00045	25	0.00047	50	2.6×10^{-4}	10	10.400
25	0.00063	40	0.00117	75	6.2×10^{-3}	20	9.896
35	0.00114			100	9.2×10^{-2}	30	9.455
45	0.002085			125	1.1	40	9.057
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 46.8$				25	9.70
		4–40 °C		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 85.6$			
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 33.36$				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 118.53$		log $K_{\text{OA}} = a + b/(T/K)$	
5–45 °C				$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 31.2$		a	–4.96
				$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 68$		b	4370
						enthalpy of phase change	
						$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 83.60$	

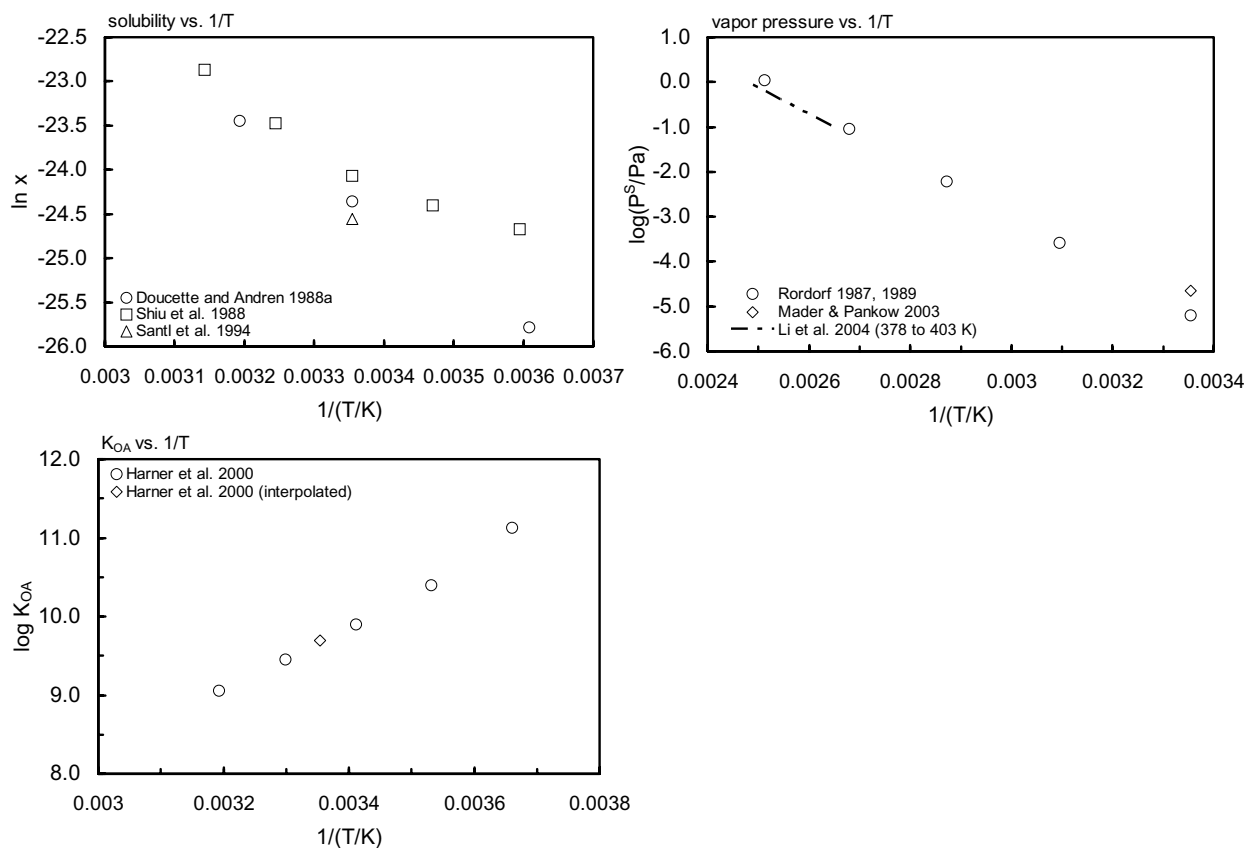
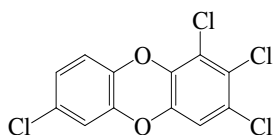


FIGURE 8.1.1.10.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4-tetrachlorodibenzo-*p*-dioxin.

8.1.1.11 1,2,3,7-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,7-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,7-TCDD

Chemical Name: 1,2,3,7-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 67028-18-6

Molecular Formula: $\text{ClC}_6\text{H}_3\text{O}_2\text{C}_6\text{HCl}_3$

Molecular Weight: 321.971

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

172–175 (Friesen et al. 1985)

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

438.3 (calculated, Rordorf 1987, 1989)

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

186.52 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

90.9 (Rordorf 1987)

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

129.41 (Rordorf 1987)

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

36.6 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

25.31 (Friesen & Webster 1990)

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

82 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S = 56 \text{ J}/\text{mol K}$), F : 0.0361 (mp at 172°C)

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

0.00042* (20°C , ^{14}C labeled, generator column-HPLC/LSC, measured range 20 – 40°C , Friesen et al. 1985)

0.00043* (20°C , generator column-HPLC/LSC, measured range 20 – 40°C , Webster et al. 1985)

0.00028 (20°C , ^{14}C labeled, generator column-HPLC/LSC, Webster et al. 1986)

0.00048* (21°C , ^{14}C -labeled, generator column-HPLC/LSC, measured range 7 – 41°C , Friesen & Webster 1990)

0.0161; 0.0131 (supercooled liquid S_L , GC-RI correlation, method, Wang & Wong 2002)

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

1.0×10^{-6} * (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1986,1989)

7.0×10^{-6} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

5.0×10^{-6} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

2.69×10^{-5} (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

$\log (P_L/\text{mmHg}) = 46.64 - 6978/(T/\text{K}) - 11.503 \cdot \log (T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

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

0.77 (calculated-P/C, Shiu et al. 1988)

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

1.15; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

- 8.19, 8.59, 8.81; 8.22, 8.60, 8.81 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 8.18, 8.60 (HPLC-RT correlation, Sarna et al. 1984)
 8.15, 7.58; 8.19, 7.72 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 6.91 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 6.48 (shake flask/slow stirring method-GC/ECD, mixture from fly-ash extract, Sijm et al. 1989a)
 8.22 (recommended, Sangster 1993)
 8.22 (recommended, Hansch et al. 1995)
 7.05 (GC-RI correlation, Wang & Wong 2002)

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

Bioconcentration Factor, log BCF:

- 3.17 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
 3.44 (fathead minnow, steady-state, wet weight, Muir et al. 1985)
 3.44, 4.44 (fathead minnow, wet wt. based, lipid based, Gobas & Schrap 1990)
 3.17, 4.17 (rainbow trout, wet wt. based, lipid based, Gobas & Schrap 1990)
 3.18, 2.90 (rainbow trout, Opperhuizen & Sijm 1990)
 3.30, 3.38 (fathead minnow, Opperhuizen & Sijm 1990)
 3.09, 3.02–3.14; 3.35, 3.30–3.37 (rainbow trout, range; fathead minnow, range, De Voogt et al. 1990)
 5.50 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

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

- 4.26 (DOC, Muir et al. 1985)
 5.39, 5.45, 5.59 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986)
 5.98, 5.97, 5.91 (20, 30, 40°C, humic acid from peat bog, Webster et al. 1986)
 6.55, 6.32, 6.44 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986)
 7.87 (sediment/water., calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

Photolysis: $t_{1/2} = 563$ min for solution photolysis in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and
 $t_{1/2} = 156$ min for surface photolysis on a clean soft glass surface under the same conditions (Nestrick et al. 1980);

first order $k = 18.13 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 10.69$ h in water-acetonitrile (2:3 v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 33.52 \times 10^2 \text{ d}^{-1}$ with direct sunlight photolysis $t_{1/2} = 2.08$ d in spring, $k = 39.41 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 1.77$ d in summer, $k = 21.77 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 3.20$ d in autumn, $k = 12.86 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 8.73$ d in winter, in aquatic bodies at latitude 40°N and $t_{1/2} = 8.73$ d averaged over full year (Choudhary & Webster 1986, 1989).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{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 of water dissolved PCDD by ozone) is $4.73 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{OH}(\text{calc}) = (16\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime of 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.0\text{--}5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 2.8–7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation: rate constant $k = 0.096 \text{ d}^{-1}$ for rainbow trout (Sijm et al. 1990).

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

$k_1 = 317 \text{ d}^{-1}$; $k_2 = 0.26 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_1 = 529 \text{ d}^{-1}$; $k_2 = 0.25 \text{ d}^{-1}$ (fathead minnow, flow-through system, Muir et al. 1985)
 $k_2 = 0.178, 0.163 \text{ d}^{-1}$ (rainbow trout, fathead minnow exposed to dioxins in their diets, Muir & Yarechewski 1988; quoted, Opperhuizen & Sijm 1990; Sijm et al. 1990)
 $k_1 = 420 \text{ to } 213 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.278 \text{ to } 0.250 \text{ d}^{-1}$ (rainbow trout exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
 $k_1 = 650 \text{ to } 408 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.322 \text{ to } 0.170 \text{ d}^{-1}$ (fathead minnow exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
 $k_2 = 9.5 \times 10^{-2}, 19.1 \times 10^{-2} \text{ d}^{-1}$ (metabolic inhibitor PBO-treated rainbow trout, control fish, 2–21 d exposure: Sijm et al. 1990)
 $k_1 = 35 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 > 0.23 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish after 120-h exposure, Sijm et al. 1993)
 $k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radical to be 0.8–2.0 d (Atkinson 1991); calculated tropospheric lifetime was 2.8–7.2 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water: direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 2.08 \text{ d}$ in spring, $t_{1/2} = 1.77 \text{ d}$ in summer, $t_{1/2} = 3.20 \text{ d}$ in fall, $t_{1/2} = 5.42 \text{ d}$ in winter, and $t_{1/2} = 8.73 \text{ d}$ averaged over a full year (Choudhary & Webster 1986);

$t_{1/2} = 10.69 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude: $t_{1/2} = 2.1 \text{ d}$ in spring, $t_{1/2} = 1.8 \text{ d}$ in summer, $t_{1/2} = 3.2 \text{ d}$ in fall and $t_{1/2} = 5.4 \text{ d}$ in winter (Choudhary & Webster 1986).

Groundwater:

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

Soil: degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ (estimated, Suzuki et al. 2000).

Biota: elimination $t_{1/2} = 2.7 \text{ d}$ (Adams et al. 1986);

$t_{1/2} = 4 \text{ d}$ in whole body of rainbow trout (Muir & Yarechewski 1988);

$t_{1/2} < 0.3 \text{ d}$ for PBO treated gold fish in 120-h exposure studies (Sijm et al. 1993).

TABLE 8.1.1.11.1

Reported aqueous solubilities and vapor pressures of 1,2,3,7-tetrachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility						Vapor pressure	
Webster et al. 1985		Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989	
generator column-HPLC/LSC		generator column-GC/ECD		gen. col.-HPLC/LSC		vapor pressure correlation	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa
20	4.30×10^{-4}	20	4.30×10^{-4}	7.0	2.43×10^{-4}	25	1.0×10^{-6}
40	1.27×10^{-3}	40	1.27×10^{-3}	11.5	2.61×10^{-4}	50	5.9×10^{-5}
				17	4.03×10^{-4}	75	1.9×10^{-3}
				21	4.80×10^{-4}	100	3.7×10^{-2}
				26	7.28×10^{-4}	125	0.57
				41	1.39×10^{-3}		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 50.68$						$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 90.9$	
25 °C						$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 129.41$	
						$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 36.6$	
						$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 82$	

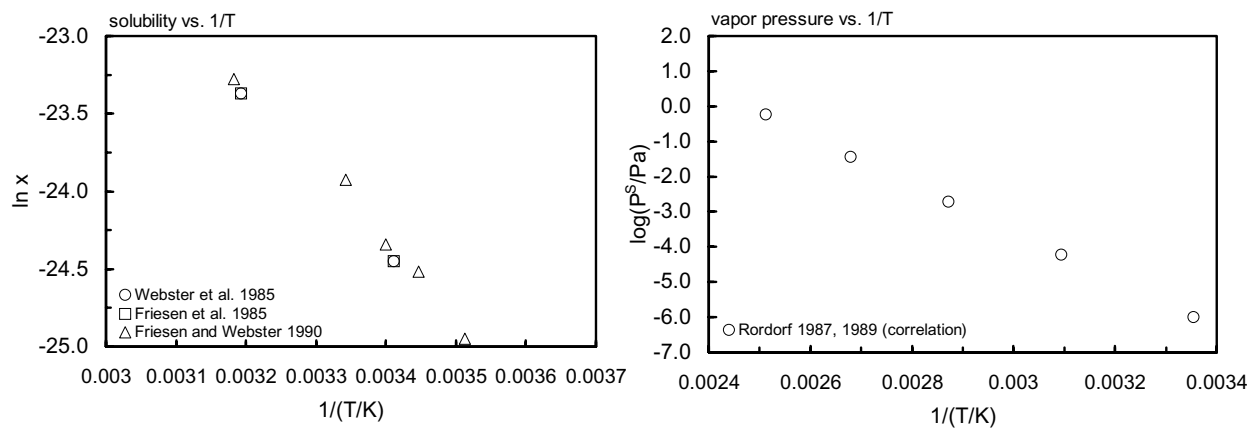
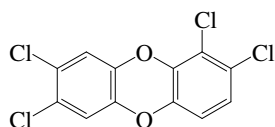


FIGURE 8.1.1.11.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,3,7-tetrachlorodibenzo-*p*-dioxin.

8.1.1.12 1,2,7,8-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,2,7,8-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,2,7,8-TCDD

Chemical Name: 1,2,7,8-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 34816-53-0

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

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

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

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

186.88 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

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

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

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

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

Water Solubility (g/m^3 or mg/L at 25°C):

0.00908 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

00223, 0.00908 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):

4.37×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

4.17×10^{-5} ; 4.37×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\log(P_L/\text{mmHg}) = 46.50 - 6956/(T/\text{K}) - 11.503 \cdot \log(T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

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

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

1.29; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

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

6.93; 6.99 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.35, 6.30, 6.30, 6.44 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

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

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

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

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

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

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

Volatilization:

Photolysis: solution photolysis $t_{1/2} = 491$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 350$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{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 of water dissolved PCDD by ozone) is $4.73 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palaushek & Scholz 1987)

$k_{OH}(\text{calc}) = 7.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.0\text{--}5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 38 \text{ L kg}^{-1} \text{ d}^{-1}$; $49 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 > 0.9 \text{ d}^{-1}$; $> 0.3 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, $104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8\text{--}2.0$ d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric lifetime $\tau(\text{calc}) = 2.8\text{--}7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

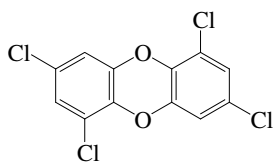
Surface water:

Groundwater:

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

Soil: degradation $t_{1/2} = 10\text{--}100$ yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} < 0.7$ d for PBO treated and $t_{1/2} < 2.1$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.13 1,3,6,8-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,3,6,8-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,3,6,8-TCDD

Chemical Name: 1,3,6,8-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 33423-92-6

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

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

219–219.5 (Pohland & Yang 1972; Rordorf 1987,1989; Delle Site 1997)

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

438.3 (calculated, Rordorf 1987, 1989)

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

192.34 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.5 (Rordorf 1987)

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

125.793 (Rordorf 1987)

118.6 (Li et al. 2004)

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

36.6 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

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

74 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S = 56 \text{ J}/\text{mol K}$), F: 0.0125 (mp at 219°C)

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

0.00032* (20°C , ^{14}C -labeled, generator column-HPLC/LSC, measured range 20 – 40°C , Webster et al. 1985)

0.000317* (20°C , ^{14}C -labeled, generator column-HPLC/LSC, measured range 20 – 40°C , Friesen et al. 1985)

0.000283, 0.000326, 0.000366, 0.000328 (^{14}C -labeled/LSC, Milli-Q treated water, lake water, simulated lake water, Milli-Q water, Servos & Muir 1989a)

0.0322 (supercooled liquid S_L , GC-RI correlation, Wang & Wong 2002)

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

0.000537* (20°C , gas saturation, measured range 20 – 100°C , Webster et al. 1985)

7.0×10^{-7} * (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1986,1987,1989)

6.76×10^{-5} (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

$\log (P_L/\text{mmHg}) = 46.99 - 6976/(T/K) - 11.503 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln (P/\text{Pa}) = 36.564 - 15127/(T/K)$, temp range 298 – 398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln (P/\text{Pa}) = (35.818 \pm 0.968) - (14262 \pm 380)/(T/K)$, temp range 378 – 408 K (Knudsen effusion technique, Li et al. 2004)

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

6.90 (23°C , batch stripping, Webster et al. 1985)

3.77 (calculated-P/C, Shiu et al. 1988)

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

1.48; 1.15 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

8.72, 9.00, 9.42; 8.72, 9.02, 9.43 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 8.70, 9.02 (HPLC-RT correlation, Sarna et al. 1984)
 8.70, 8.08; 8.70, 8.12 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 7.20, 7.13 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 7.13 (corrected HPLC-RT value, Burkhard & Kuehl 1986)
 6.29 (shake flask/slow stirring method-GC/MS, Sijm et al. 1989a)
 7.18 (recommended, Sangster 1993)
 6.29 (recommended, Hansch et al. 1995)
 6.79 (GC-RI correlation, Wang & Wong 2002)

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

Bioconcentration Factor, log BCF:

3.03, 2.67 (fathead minnow, rainbow trout, Corbet et al. 1983, 1988)
 3.39 (rainbow trout, steady-state, wet weight basis, Muir et al. 1985)
 3.83 (fathead minnow, steady-state, wet weight basis, Muir et al. 1985)
 3.39, 3.83 (rainbow trout average, fathead minnow average, Muir et al. 1986)
 3.39, 3.32, 3.57 (*Oncorhynchus mykiss*, Servos et al. 1989)
 1.08–3.75, 2.14, 1.76–1.93 (Amphipod in lake water, in simulated lake water, in water with Aldrich humic acid, Servos & Muir 1989a)
 4.20, 4.20 (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)
 5.00 (goldfish after 6 d exposure: metabolic inhibitor PBO-treated, Sijm et al. 1989b)
 3.76, 3.54–3.90; 3.32, 3.23–3.40 (fathead minnow, range; rainbow trout, range, De Voogt et al. 1990)
 3.83, 4.83 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 3.39, 4.39 (rainbow trout, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 3.46, 3.30, 3.15 (quoted, rainbow trout exposed to different concentrations, Opperhuizen & Sijm 1990)
 3.76, 3.75 (fathead minnow exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
 3.70 (10.1 ng/L for 0–10 d, predicted for biota held in lake enclosures, Servos et al. 1992b)
 3.12 (17.7 ng/L for 0–10 d, invertebrates, Servos et al. 1992b)
 3.20 (21.4 ng/L for 0–10 d, unionid clams & white suckers gill, Servos et al. 1992b)
 2.36 (3.1 ng/L for 0–10 d, white suckers carcass, Servos et al. 1992b)
 3.21 (1.6 ng/L for 14–24 d, invertebrates, Servos et al. 1992b)
 2.95 (0.9 ng/L for 14–24 d, unionid clams, Servos et al. 1992b)
 3.32 (2.1 ng/L for 14–24 d, white suckers gill, Servos et al. 1992b)
 2.70 (1.0 ng/L for 14–24 d, white suckers carcass, Servos et al. 1992b)
 4.54 (3.5 ng/L for 0–104 d, white suckers gill, Servos et al. 1992b)
 4.26 (1.8 ng/L for 0–104 d, white suckers carcass, Servos et al. 1992b)
 3.13 (gold fish, PBO-treated, 120-h exposure, Sijm et al. 1993)
 5.53 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} :

4.36 (DOC, De Voogt et al. 1990)
 6.74 (calculated- K_{ow} , Corbet et al. 1988)
 2.11–3.75, 2.39, 2.05–2.38 (DOC partition coeff., lake water, simulated lake water, Aldrich humic acid, Servos & Muir 1989a)
 5.98–6.23 (sediment, Servos & Muir 1989b)
 7.50 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 6.23 (derived from soot-water distribution coeff., Barring et al. 2002)

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

Volatilization: 3.9 d in water of 0.5 m depth in a small pond (Corbet et al. 1988)

Photolysis: solution photolysis $t_{1/2} = 507$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis on a clean glass surface under the same conditions with $t_{1/2} = 264$ min (Nestrick et al. 1980; quoted, Muto et al. 1991);

first-order $k = 59.57 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 0.35$ d in spring, $t_{1/2} = 0.31$ d in summer, $t_{1/2} = 0.53$ d in fall, $t_{1/2} = 0.84$ d in winter and $t_{1/2} = 1.47$ d averaged over full year (Choudhary & Webster 1986; quoted, Muto et al. 1991)

$t_{1/2} = 14.0\text{--}28.5$ h in outdoor pool and $t_{1/2} = 6.3\text{--}8.0$ d in natural water in a Pyrex flask under sunlight (Corbet et al. 1988)

$t_{1/2} = 25$ h in water column (Corbet et al. 1983)

$t_{1/2} = 6.3\text{--}8.0$ d for natural water under sunlight and photodegradation $t_{1/2} = 0.3$ d in summer sunlight at 40°N and $t_{1/2} = 7$ d in a 1-L flask (Corbet et al. 1988)

photolysis $k = 59.57 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 3.24$ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 198.13 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 0.35$ d in spring, $k = 226.99 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 0.31$ d in summer, $k = 130.91 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 0.53$ d in fall, $k = 82.85 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 0.84$ d in winter; while experimentally determined sunlight photolysis $t_{1/2} = 3.5$ d for ^{14}C labeled 1,3,6,8-TCDD in pond water (Choudhary & Webster 1989)

$t_{1/2} = 78.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

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

photooxidation may be an important path of transformation (Corbet et al. 1988)

k (oxidative degradation rate of water dissolved PCDD by ozone) is $3.21 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = (16\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (7.6\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.0\text{--}5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 184 \text{ d}^{-1}$; $k_2 = 0.10 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_1 = 574 \text{ d}^{-1}$; $k_2 = 0.10 \text{ d}^{-1}$ (fathead minnow, Muir et al. 1985; quoted, Adams et al. 1986)

$k_1 = 225, 221, 106 \text{ d}^{-1}$ (rainbow trout fry, exposed to concn of 4, 74, 211 ng/L, 5-d uptake study, Muir et al. 1986)

$k_2 = 0.074, 0.110, 0.111 \text{ d}^{-1}$ (rainbow trout fry, exposed to 4, 74, 211 ng/L, 24 to 48-d depuration study, Muir et al. 1986)

$k_1 = 526, 621 \text{ d}^{-1}$ (fathead minnow, exposed to concn of 10, 41 ng/L, 5-d uptake study, Muir et al. 1986)

$k_2 = 0.08, 0.122 \text{ d}^{-1}$ (fathead minnow, exposed to concn of 10, 41 ng/L, 24 to 48-d depuration study, Muir et al. 1986)

$k_1 = 225, 97 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)

$k_2 = 0.211 \text{ d}^{-1}$ (fathead minnow, calculated, Corbet et al. 1983; quoted, Opperhuizen & Sijm 1990)

$k_2 = 0.158 \text{ d}^{-1}$ (rainbow trout, calculated, Corbet et al. 1983; quoted, Opperhuizen & Sijm 1990)

$k_1 = 225, 221, 106 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.074, 0.110, 0.110 \text{ d}^{-1}$ (rainbow trout exposed to different concentrations in a flow system, quoted, Opperhuizen & Sijm 1990)

$k_1 = 526, 621 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.080, 0.122 \text{ d}^{-1}$ (fathead minnow exposed to different concentrations in a flow system, quoted, Opperhuizen & Sijm 1990)

$k_1 = 1200 \text{ d}^{-1}$; $k_2 = 0.06 \text{ d}^{-1}$ (filter-feeder, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

$k_1 = 285 \text{ d}^{-1}$; $k_2 = 0.12 \text{ d}^{-1}$ (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

$k_1 = 142, 116 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.14, > 0.24 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8\text{--}2.0 \text{ d}$ calculated for a tetra-chlorinated dioxin based on the gas-phase reaction rate with OH radicals (Atkinson 1991);

calculated tropospheric lifetime $\tau = 2.8\text{--}7.2 \text{ d}$ for with OH radical (Kwok et al. 1995).

Surface water: direct sunlight photolysis in aquatic bodies at latitude 40°N for various seasons with half-lives: 0.35 d in spring, 0.31 d in summer, 0.53 d in fall, 0.84 d in winter and 1.47 d averaged over full year (Choudhary & Webster 1986);

$t_{1/2} = 14.0\text{--}28.5 \text{ h}$ for outdoor pool and $t_{1/2} = 6.3\text{--}8.0 \text{ d}$ for natural water in a Pyrex flask under sunlight (Corbet et al. 1988);

$t_{1/2} = 3.24 \text{ h}$ for photolysis in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude calculated to be: $t_{1/2} = 0.35 \text{ d}$ in spring, $t_{1/2} = 0.31 \text{ d}$ in summer, $t_{1/2} = 0.53 \text{ d}$ in fall, and $t_{1/2} = 0.84 \text{ d}$ in winter (Choudhary & Webster 1989);

calculated transformation rate constant in simulated lake enclosure of $9.4 \times 10^{-2} \text{ h}^{-1}$ (Servos et al. 1992a).

Groundwater:

Sediment: $t_{1/2} = 51.2\text{--}69.2 \text{ d}$ (Corbet et al. 1988);

calculated $t_{1/2} = 10 \text{ yr}$ with a transformation rate constant $k = 7.9 \times 10^{-6} \text{ h}^{-1}$ (Servos et al. 1992a);

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

Soil: degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ (estimated, Suzuki et al. 2000).

Biota: $t_{1/2} = 4 \text{ d}$ in rainbow trout (Neely 1979; quoted, Niimi & Oliver, 1983,1986);

$t_{1/2} = 4 \text{ d}$ in rainbow trout (Corbet et al. 1983; quoted, Niimi & Oliver 1986);

$t_{1/2} = 2 \text{ d}$ in rainbow trout (Muir et al. 1984);

$t_{1/2} = 6\text{--}9 \text{ d}$ for both rainbow trout fry and fathead minnow (Muir et al. 1986);

$t_{1/2} = 6.90 \text{ d}$ in fathead minnow (Adams et al. 1986);

$t_{1/2} = 41 \text{ to } 44 \text{ d}$ in rooted vegetable (Corbet et al. 1988);

$t_{1/2} = 15 \text{ d}$ in whole body of rainbow trout (Muir et al. 1990);

half-lives in gold fish: $t_{1/2} = 4.8 \text{ d}$ for PBO treated and $t_{1/2} < 0.3 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993)

TABLE 8.1.1.13.1

Reported aqueous solubilities and vapor pressures of 1,3,6,8-tetrachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure			
Webster et al. 1985		Friesen et al. 1985		Webster et al. 1985		Rordorf 1987, 1989	
generator column-HPLC/LSC		generator column-GC/ECD		gas saturation-GC		vapor pressure correlation	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
20	3.20×10^{-4}	20	3.20×10^{-4}	20	5.37×10^{-4}	25	7.0×10^{-7}
40	3.90×10^{-3}	40	3.90×10^{-3}	50	1.32×10^{-3}	50	3.6×10^{-5}
				100	1.12×10^{-2}	75	1.0×10^{-3}
						100	1.9×10^{-2}
						125	0.24
				$\Delta H_v/(\text{kJ mol}^{-1}) = 86.5$			
				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 125.794$			
				$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 36.6$			
				$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 74$			

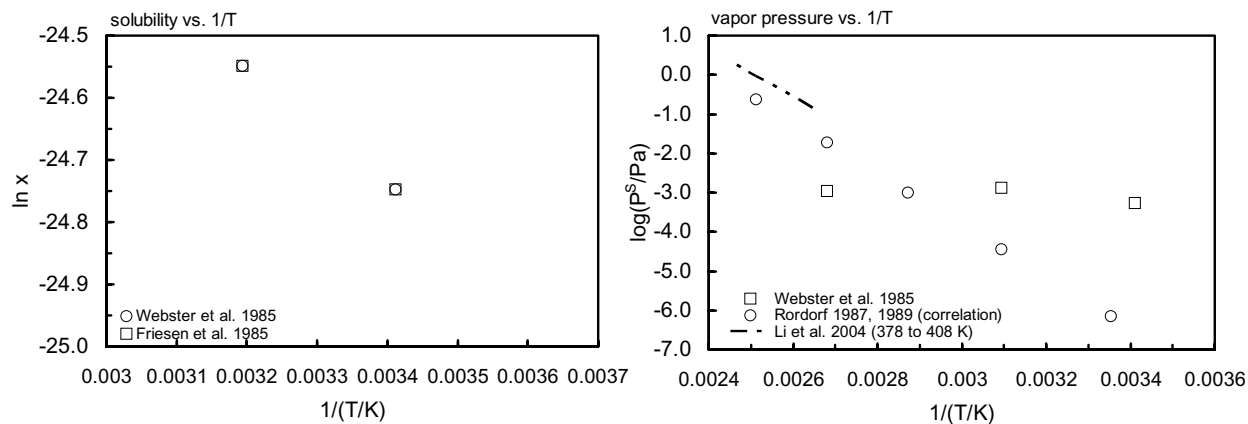
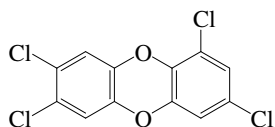


FIGURE 8.1.1.13.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,3,6,8-tetrachlorodibenzo-*p*-dioxin.

8.1.1.14 1,3,7,8-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,3,7,8-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,3,7,8-TCDD

Chemical Name: 1,3,7,8-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 50585-46-1

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

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

193.5–195 (Rordorf 1986, 1987, 1989)

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

438.3 (calculated, Rordorf 1986, 1987, 1989)

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

188.33 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.9 (Rordorf 1987)

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

127.77 (Rordorf 1987)

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

36.6 (Rordorf 1987)

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

78 (Rordorf 1986, 1987, 1989)

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

Water Solubility (g/m^3 or mg/L at 25°C):

0.0203 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

00223, 0.0203 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

8.4×10^{-7} , 4.5×10^{-5} , 1.4×10^{-3} , 2.6×10^{-2} , 0.35 (25, 50, 75, 100, 125°C , predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

8.32×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

4.17×10^{-5} ; 8.32×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\log(P_L/\text{mmHg}) = 46.80 - 6977/(T/\text{K}) - 11.503 \cdot \log(T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

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

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

1.29; 1.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

6.93; 6.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.30; 6.29, 6.28, 6.40, 6.44 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

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

Bioconcentration Factor, $\log BCF$:

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

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

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

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

Volatilization:

Photolysis: solution photolysis $t_{1/2} = 153$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 160$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

$t_{1/2} = 86.6$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

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

$k_{OH}(\text{calc}) = 13 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.0 - 5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d at for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 57 \text{ L kg}^{-1} \text{ d}^{-1}$; $99 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.14 \text{ d}^{-1}$; $> 0.24 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, $104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8\text{--}2.0$ d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

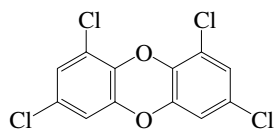
Surface water:

Groundwater:

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

Soil: degradation $t_{1/2} = 10\text{--}100$ yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 2.1$ d for PBO treated and $t_{1/2} < 0.4$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.15 1,3,7,9-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,3,7,9-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,3,7,9-TCDD

Chemical Name: 1,3,7,9-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 62470-53-5

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

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

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

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

192.34 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

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

123.6 (Li et al. 2004)

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

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

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

Water Solubility (g/m^3 or mg/L at 25°C):

0.0294 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

00294, 0.0294 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

5.50×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

5.89×10^{-5} ; 5.50×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\log(P_L/\text{mmHg}) = 46.86 - 6956/(T/\text{K}) - 11.503 \cdot \log(T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/\text{Pa}) = (37.221 \pm 0.469) - (14864 \pm 185)/(T/\text{K})$; temp range 383–408 K (Knudsen effusion technique, Li et al. 2004)

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

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

1.42; 0.589 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

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

6.83; 6.68 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.28, 6.12, 6.47, 6.44 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

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

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

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

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

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

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

Volatilization:

Photolysis: solution photolysis $t_{1/2} = 499$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 169$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

$t_{1/2} = 79.7$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

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

$k_{OH}(\text{calc}) = (16 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.0\text{--}5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 54 \text{ L kg}^{-1} \text{ d}^{-1}$, $98 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1 \text{ d}^{-1}$, $> 2.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, $104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8\text{--}2.0$ d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

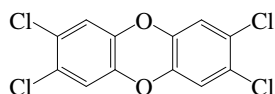
Surface water:

Groundwater:

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

Soil: degradation $t_{1/2} = 10\text{--}100$ yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} > 7$ d for PBO treated and $t_{1/2} < 0.3$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.16 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin

Common Name: 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin

Synonym: 2,3,6,7-tetrachlorodibenzo-*p*-dioxin, TCDD, TCDBD, 2,3,6,7- TCDD, 2,3,7,8-TCDD, dioxin

Chemical Name: 2,3,7,8-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 1746-01-6

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

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

295 (Lide 2003)

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

421.2 (Schroy et al. 1985a)

Density (g/cm^3 at 20°C):

1.827 (solid at 25°C , Boer et al. 1972; Schroy et al. 1985a)

1.021 (liquid at normal boiling point, Schroy et al. 1985a)

Molar Volume (cm^3/mol):

184.32, 184.97 (calculated-liquid density, crystalline volume, Govers et al. 1990)

188.34 (liquid molar volume, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

71.71 (at normal bp, Schroy et al. 1985a)

79.9 (Rordorf 1987)

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

123.91 (Schroy et al. 1985b)

124.001 (Rordorf 1987)

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

38.91 (Boer et al. 1972; Schroy et al. 1985a,b; Ruelle & Kesselring 1997)

38.9, 36.6 (Obs., predicted, Rordorf 1986, 1987)

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

69 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.00244 (mp at 295°C)

0.0017 (Shiu et al. 1988)

4.07×10^{-4} (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):

0.0002 (shake flask-GC/ECD, Crummett & Stehl 1973)

3.17×10^{-4} (^{14}C -labeled, generator column-HPLC/LSC, Webster et al. 1983)

1.93×10^{-5} (shake flask-GC/MS, Marple et al. 1986a)

7.91×10^{-6} (^{14}C -labeled, Adams & Blaine 1986)

1.29×10^{-5} , 4.83×10^{-4} (4.3, 17.3°C , generator column-GC/MS, Lodge 1989)

$\log [S_L/(\text{mol}/\text{L})] = 0.190 - 2089/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)

0.0158 (supercooled liquid S_L , GC-RI correlation, Wang & Wong 2002)

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

1.0×10^{-7} (^{14}C -gas saturation method, Jaber & Podoll 1983)

$(4.50 \pm 2) \times 10^{-6}$ (gas saturation-GC, Rordorf 1985a)

$(3.5-6.3) \times 10^{-6}$, $(1.3-3.1) \times 10^{-4}$, $(2.8-8.9) \times 10^{-2}$, $(3.9-15.9) \times 10^{-2}$, $(4.4-21.9) \times 10^{-1}$ (25, 50, 75, 100, 125°C , predicted using estimated ΔH_{sub} and ΔS_{sub} for tetra-chloro isomers, Rordorf 1985a)

$4.61 \times 10^{-7*}$ (30.1°C , gas saturation-GC/MS, measured range $30.1-71.1^{\circ}\text{C}$ Schroy et al. 1985a,b)

$\log (P/\text{mmHg}) = 12.89784 - 6477.132/(273.15 + t/^{\circ}\text{C})$; temp range $10-305^{\circ}\text{C}$ (Antoine eq., from gas saturation-GC/MS, Schroy et al. 1985b)

$\log (P/\text{mmHg}) = 8.78307 - 4098.173/(273.15 + t/^{\circ}\text{C})$; temp range 305–420 $^{\circ}\text{C}$ (Antoine eq., from gas saturation-GC/MS, Schroy et al. 1985b)
 $2.02 \times 10^{-7*}$, 4.60×10^{-7} , 9.65×10^{-6} , 4.58×10^{-5} , 1.59×10^{-4} (25, 30, 50, 62, 71 $^{\circ}\text{C}$, results derived from Antoine eq., gas saturation-GC/MS, Schroy et al. 1985b)
 $\ln (P/\text{Pa}) = 34.570834 - [14903.438/(T/\text{K})]$, temp range: 283.15–578.15 K (gas saturation, Schroy et al. 1985a)
 $\ln (P/\text{Pa}) = 25.104351 - 93430.391/(T/\text{K})$, temp range: 578.15–703.15 K (gas saturation, Schroy et al. 1985a)
 $8.71 \times 10^{-6*}$ (20 $^{\circ}\text{C}$, gas saturation-LSC, measured range 20–100 $^{\circ}\text{C}$, Webster et al. 1985)
 9.87×10^{-8} (^{14}C -gas saturation, Podoll et al. 1986)
 8.14×10^{-8} , 6.0×10^{-5} (20 $^{\circ}\text{C}$, quoted: solid P_s , supercooled liquid P_L , Bidleman & Foreman 1987)
 $2.0 \times 10^{-7*}$ (gas saturation-GC, measured range 25–125 $^{\circ}\text{C}$, Rordorf 1987, 1989)
 6.20×10^{-7} , 2.6×10^{-5} , 6.1×10^{-4} , 9.7×10^{-3} , 1.1×10^{-1} (25, 50, 75, 100, 125 $^{\circ}\text{C}$, predicted-vapor pressure correlation method, Rordorf 1987, 1989)
 6.17×10^{-4} ; 2.51×10^{-7} (supercooled liquid P_L ; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)
 $\log (P_s/\text{Pa}) = 12.66 - 5739/(T/\text{K})$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 9.05 - 3663/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)
 1.17×10^{-4} ; 5.75×10^{-5} (supercooled liquid P_L , quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 $\log (P_s/\text{Pa}) = 15.0391 - 6482.7/(T/\text{K})$; temp range 5–50 $^{\circ}\text{C}$ (regression eq. from literature data, Shiu & Ma 2000)
 5.25×10^{-4} (supercooled liquid P_L , Harner et al. 2000)
 2.57×10^{-5} ; 5.75×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
 5.56×10^{-7} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)
 3.35×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$, Mader & Pankow 2003)
 $\log (P_L/\text{mmHg}) = 49.89 - 6705/(T/\text{K}) - 12.569 \cdot \log (T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

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

0.0021 (calculated-P/C, Mabey et al. 1982)
 0.152 (calculated-P/C, Crosby 1985)
 0.212 (calculated-P/C, Schroy et al. 1985)
 1.64 (calculated-P/C, Podoll et al. 1986)
 1.63, 3.34, 10.34 (calculated-P/C, Shiu et al. 1988)
 7.93 (calculated-P/C, Jury et al. 1990)
 1.62 (calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 8.86 - 1574/(T/\text{K})$ (Passivirta et al. 1999)
 1.12; 1.62 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

5.38 (Crummett & Stehl 1973)
 6.19 (Neely 1979; Veith et al. 1979; Corbet et al. 1983)
 6.15 (Kenaga 1980;)
 8.93 (HPLC-RT correlation, Sarna et al. 1984)
 7.02 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 6.64 (shake flask-GC/MS, Marple et al. 1986b)
 6.42 (shake flask/slow stirring method-GC/MS, Sijm et al. 1989a)
 7.02 (recommended, Sangster 1993)
 6.53 (recommended, Hansch et al. 1995)
 7.06 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25 $^{\circ}\text{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

9.70 (calculated- $K_{\text{OW}}/K_{\text{AW}}$, Wania & Mackay 1996)
 10.05*; 9.91 (generator column-GC; calculated, Harner et al. 2000)
 11.04 (7 $^{\circ}\text{C}$, GC-retention time correlation, Harner et al. 2000)
 $\log K_{\text{OA}} = -6.19 + 4840/(T/\text{K})$; temp range 10–50 $^{\circ}\text{C}$ (generator column-GC/ECD, Harner et al. 2000)
 9.95 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 1.69, 2.34, 2.08 (*daphnia*, ostracod, brine shrimp, ^{14}C -labeled-LSC, Matsumura & Benezet 1973)
 4.30–4.41; 3.6–3.95 (snail, *gambusia*, *daphnids*; duckweed, algae, catfish; Isensee & Jones 1975)
 3.96 (rainbow trout, Branson et al. 1985)
 3.90 (fathead minnow, steady-state, wet weight, Adams et al. 1986)
 3.73, 4.55 (fish: flowing water test, static ecosystem test, Kenaga & Goring 1980, Kenaga 1980)
 3.97 (rainbow trout, Branson et al. 1983)
 3.97, 3.67 (rainbow trout: whole body, muscle, Branson et al. 1985)
 1.38–1.60 (rhesus monkey, Geyer et al. 1986)
 4.11 (guppy, Opperhuizen et al. 1986)
 4.43, 4.59 (rainbow trout: measured average, estimated BCF at steady-state, for 28-d exposure, Mehrle et al. 1988)
 4.30, 5.0 (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)
 3.89, 4.59 (fathead minnow, rainbow trout, De Voogt et al. 1990)
 5.80, 5.90 (goldfish after 6 d exposure: PBO-treated, control, Sijm et al. 1989b)
 4.11, 5.64 (guppy, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 3.97, 4.70; 4.97, 5.70 (rainbow trout, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 4.63, 4.40 (pine needle/air BCF values, Reissinger et al. 1989)
 4.59, 4.58, 4.93, 4.57, 3.97 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
 4.11, 3.90, 3.78 (guppy, fathead minnow, mosquito fish, quoted, Opperhuizen & Sijm 1990)
 2.62 (human, Webster & Connett 1991)
 5.24; 4.91 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 5.24; 4.83; 5.02 (guppies, 21-d exposure, lipid wt basis: measured- $C_{\text{fish}}/C_{\text{W}}$; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 5.24; 5.48 (lipid wt. base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 5.71, 6.71 (fish medaka 10% lipid: BCF_{W} , BCF_{L} , Geyer et al. 2000)
 6.02, 6.05 (fish muscle log BCF_{L} calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 5.67 (organic carbon soil, calculated- K_{OW} , Kenaga 1980)
 6.95, 7.39–7.58 (calculated- K_{OW} , 10 soils from Missouri & New Jersey, Jackson et al. 1985)
 6.22–6.54; 5.96–6.09 (red clay soil from Missouri, Alluvial soil from Missouri, Marple et al. 1986)
 4.83 (hydroxy aluminum-clay, Srinivasan & Fogler 1987)
 6.60 (^{14}C -labeled, soil, batch equilibrium-sorption isotherm, GC/ECD, Walters & Guiseppi-Elie 1988)
 3.06 (soil, Eduljee 1987)
 6.30; 7.59; 7.25 (Lake Ontario sediment; solids; DOC dissolved organic carbon; batch equilibrium-sorption isotherm, Lodge & Cook 1989)
 6.24, 6.10, 5.10 (Eglin Air Force Base soil/water with 0.01% surfactant from Florida at pH 4, 7, 8.5, batch equilibrium-GC, Puri et al. 1989)
 6.50, 5.86, 4.81 (Time Beach soil/water with 0.01% surfactant from Missouri at pH 4, 7, 8.5, Puri et al. 1989)
 5.70, 5.09, 4.76 (Visalia soil/water with 0.01% surfactant from California at pH 4, 7, 8.5, Puri et al. 1989)
 6.44, 6.66 (batch equilibrium-sorption isotherms: 2-d, 10-d isotherm, regression analysis for sorption of uncontaminated Time Beach soil from water, Walters et al. 1989)
 6.14 (soil, Jury et al. 1990)
 6.80 (Baltic sea particulate filed samples, concn distribution-GC/MS, Broman et al. 1991)

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

Volatilization: probably not an important process (Callahan et al. 1979)

$t_{1/2} = 20\text{--}200$ d from water column which will be slowed down further by the fact that it is sorbed to the sediment and biota (Mill 1985)

$t_{1/2} \sim 32$ d for ponds and $t_{1/2} \sim 16$ d for rivers (Podoll et al. 1986)

$t_{1/2} = 104$ d from soil by calculation assuming diffusion of TCDD in soil is vapor-dominated up to volumetric water content of $0.3 \text{ m}^3/\text{m}^3$, and then liquid-dominated to saturation (Eduljee 1987)

$t_{1/2} = 190$ d (Thibodeaux & Lipsky 1985; quoted, Eduljee 1987)

$t_{1/2} = 365$ d for volatilization from below surface soil (Jury et al. 1990)

$k = 0.0054 \text{ h}^{-1}$ with $t_{1/2} = 128$ h from grass foliage (McCrary & Maggard 1993)

Photolysis:

stable to sunlight for at least 14 d in distilled water (Crosby et al. 1971; quoted, Dougherty et al. 1991)

$t_{1/2} = 3$ h in methanol solution in sunlight (Plimmer et al. 1973)

$t_{1/2} = 56$ min for vapor in sunlight (Peterson 1976; quoted, Mill 1985)

thin film of TCDD on glass plates showed transformation at about 6 h (Crosby & Wong 1977);

$t_{1/2}(\text{soln}) = 56.8$ min in *n*-hexadecane on a clean soft glass surface at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 140$ h on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984; Dougherty et al. 1991)

TCDD extracted from the aqueous sludge with hexane can be continuously degraded by a mercury arc of UV radiation (Exner et al. 1982; quoted, Crosby 1985)

$t_{1/2} \sim 1$ d in water, $t_{1/2} = 0.1$ d in vapor and $t_{1/2} = 1\text{--}100$ d in soil with $t_{1/2} = 50$ d for a small fraction in water column in equilibrium with sediment sorbed with TCDD (Mill 1985)

$k_p = 6.94 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 27$ h in a 90:10 mixture of distilled water and acetonitrile under summer sunlight; $k_p = 0.15 \text{ d}^{-1}$ with $t_{1/2} = 6$ d in summer sunlight at 40°L surface waters (Dulin et al. 1986)

$t_{1/2} = 81$ h after adjusting for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)

$k = 0.14 \text{ d}^{-1}$ with $t_{1/2} = 118$ h in winter, $k = 0.61 \text{ d}^{-1}$ with $t_{1/2} = 27$ h in spring, $k = 0.78 \text{ d}^{-1}$ with $t_{1/2} = 21$ h in summer, and $k = 0.32 \text{ d}^{-1}$ with $t_{1/2} = 51$ h in autumn for aqueous dissolved TCDD in sunlight over four seasons at 40°N latitude (Podoll et al. 1986)

photodegradation $t_{1/2} = 10$ min, a very rapid process at soil surface during the day (Facchetti et al. 1986)

$t_{1/2} = 14$ min sunlight induced photolysis in isooctane solution and sunlight induced solid phase $t_{1/2} = 300$ h dispersed as solid films (Buser 1988)

$k = 5.9 \times 10^{-3} \text{ s}^{-1}$ rate constant for photolysis in air at 150–350°C (Orth et al. 1989)

$k = 0.15 \text{ min}^{-1}$ first-order photolysis rate constant in isooctane and over 90% was lost in 21 min of irradiation in isooctane whereas only greater than 55% TCDD remained in soil after 15 d of irradiation (Kieatiwong et al. 1990)

photolytic degradation $t_{1/2} = 4.5$ h in extract from fly ash exposed to UV light from a distance of 20 cm for native congener and $t_{1/2} = 5.2$ h for ^{13}C -labeled congener in tetradecane solution (Tysklind & Rappe 1991)

$t_{1/2} = 31$ min in hexadecane and $t_{1/2} = 27$ min in ethyl oleate (Dougherty et al. 1991)

photodegradation $k = 0.0156 \text{ h}^{-1}$ with $t_{1/2} = 44$ h for TCDD sorbed to grass foliage and exposed to natural sunlight (McCrary & Maggard 1993)

$t_{1/2} = 52$ h, direct sunlight photolysis in water-acetonitrile in midday of mid-summer at 40°N (quoted, Zepp 1991)

$t_{1/2} = 55.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

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

$k = 6 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 320$ h, estimated for the reaction with 3×10^{-15} mole OH radicals in vapor phase (Singh 1977; quoted, Mill 1985)

laboratory tests shown that 99.5% TCDD was oxidized in 21 s at 800°C while only 50% reacted at 700°C (Esposito et al. 1980; quoted, Crosby 1985)

$k_{\text{OH}} = 2 \times 10^8 \text{ mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 13$ d for oxidation in vapor phase (Mill 1985)

$k_{\text{OH}} > 1.0 \times 10^8 \text{ mol}^{-1} \text{ s}^{-1}$, $1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 200$ h (Podoll et al. 1986)

$k_{\text{OH}}(\text{calc}) = 9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an atmospheric lifetime $\tau \sim 3$ d (Atkinson 1987a)

$k_{\text{OH}}(\text{calc}) = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship Atkinson 1987b)

photooxidation $t_{1/2} = 22.3\text{--}223$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k = 1.33 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$, the oxidative degradation of water dissolved TCDDs by ozone takes place only under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 7.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ at room temp. (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous solutions (Haag & Yao 1992)

$k_{\text{OH}}(\text{calc}) = (2.0 - 5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2 \text{ d}$ for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis: hydrolysis is not likely under environmental conditions (Callahan et al. 1979; Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 10032 \text{ h}$, based on soil die-away test data (Kearney et al. 1971; quoted, Howard et al. 1991) and $t_{1/2} = 14160 \text{ h}$, based on lake water and sediment dieaway test data (Ward & Matsumura 1978; quoted, Howard et al. 1991)

$t_{1/2} > 1.0 \text{ yr}$ (Callahan et al. 1979);

$t_{1/2}(\text{aq. anaerobic}) = 40128\text{--}56640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

$k_1 = 4.64 \text{ mL g}^{-1} \text{ h}^{-1}$; $k_2 = 5.00 \times 10^{-4} \text{ h}^{-1}$ (rainbow trout, Neely 1979)

$k_1 = 108 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.012 \text{ d}^{-1}$ (rainbow trout, Branson et al. 1983, 1985)

$k_1 = 476 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.120 \text{ d}^{-1}$ (fathead minnow, Adams et al. 1986)

$k_1 = 600 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.046 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1986)

$k_1 = 1832, 1543, 1337, 1591 \text{ d}^{-1}$ and $k_2 = 0.047, 0.041, 0.015, 0.043 \text{ d}^{-1}$ (rainbow trout, exposed to 38 pg/L, 176 pg/L, 382 pg/L, 702 pg/L for 28 d, Mehrle et al. 1988)

$k_1 = 216, 604 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)

$k_2 = 0.008 \text{ d}^{-1}$ (rainbow trout, quoted, Opperhuizen & Sijm 1990)

$k_1 = 381 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.048 \text{ d}^{-1}$ (fathead minnow, quoted, Opperhuizen & Sijm 1990)

$k_1 = 100 \text{ mL g}^{-1} \text{ d}^{-1}$ (mosquito fish, quoted, Opperhuizen & Sijm 1990)

$k_1 = 86 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish, 120-h exposure, metabolic inhibitor PBO-treated; Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 > 1.3 \text{ d}^{-1}; < 0.1 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated; control, Sijm et al. 1993)

$k_1 = 500 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.049 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0061 \text{ d}^{-1}$ with a biological $t_{1/2} = 49 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_2 = 0.0246 \text{ d}^{-1}$ with $t_{1/2} = 28 \text{ d}$ (newly contaminated oysters, Gardinali et al. 2004)

$k_2 = 0.0199 \text{ d}^{-1}$ with $t_{1/2} = 35 \text{ d}$ (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: dominant transformation process in the atmosphere (Atkinson et al. 1982)

$t_{1/2} = 200 \text{ h}$ for reaction with OH radical (Podoll et al. 1986)

atmospheric lifetime of $\sim 3 \text{ d}$ at room temp. (Atkinson 1987a)

$t_{1/2} = 22.3\text{--}223 \text{ h}$, based on estimated photooxidation half-life in air (Howard et al. 1991)

$t_{1/2} = 1 \text{ h}$, an upper limit, undergo rapid photolysis in vapor phase (Travis & Hattemer-Frey 1987)

atmospheric $k = 0.012 \text{ min}^{-1}$ with $t_{1/2} = 58 \text{ min}$ in summer sunlight at 40°N latitude (Buser 1988)

reaction rate constant $k \sim 0.02 \text{ h}^{-1}$ (Paterson et al. 1990)

tropospheric lifetime $\tau(\text{calc}) = 0.8\text{--}2.0 \text{ d}$ for reaction with OH radical (Atkinson 1991)

tropospheric lifetime $\tau(\text{calc}) = 2.8\text{--}7.2 \text{ d}$ for with OH radical (Kwok et al. 1995);

$t_{1/2} = 200 \text{ h}$ at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis $t_{1/2} = 3 \text{ h}$ in methanol solution under sunlight (Plimmer et al. 1973);

$t_{1/2} = 600 \text{ d}$ in a model aquatic environment (Ward & Matsumura 1978);

reaction rate constant estimated to be $2.6 \times 10^{-5} \text{ h}^{-1}$ (Mackay et al. 1985);

calculated sunlight photolysis half-lives over four seasons at 40°N latitude averaged over for 24 h exposure per day: $t_{1/2} = 130 \text{ h}$ in winter, $t_{1/2} = 28 \text{ h}$ in spring, $t_{1/2} = 20 \text{ h}$ in summer and $t_{1/2} = 52 \text{ h}$ in fall (Mill et al. 1982; quoted, Mill 1985);

calculated photolysis half-lives in sunlight at 40°N latitude: $t_{1/2} = 118 \text{ h}$ in winter, $t_{1/2} = 27 \text{ h}$ in spring, $t_{1/2} = 21 \text{ h}$ in summer and $t_{1/2} = 51 \text{ h}$ in fall (Podoll et al. 1986);

photolysis $t_{1/2} = 40 \text{ h}$ in near-surface waters is an important degradative pathway (Travis & Hattemer-Frey 1987);

$t_{1/2} = 14 \text{ min}$, sunlight-induced photolysis half-life in isooctane (Buser 1988);

reaction rate constant estimated to be 0.008 h^{-1} (Paterson et al. 1990);

- photolysis $t_{1/2} = 27\text{--}81$ h, aerobic $t_{1/2} = 1.15\text{--}1.62$ yr, anaerobe $t_{1/2} = 4.58\text{--}6.45$ yr (Howard et al. 1991)
 $t_{1/2} = 4000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
- Groundwater: $t_{1/2} = 20064\text{--}28320$ h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).
- Sediment: $t_{1/2} = 12000\text{--}14400$ h in aquatic sediment (Ward & Matsumura 1978; quoted, Quensen & Matsumura 1983)
 reaction rate constant $k \sim 8.0 \times 10^{-6} \text{ h}^{-1}$ (Mackay et al. 1985)
 $k \sim 1.5 \times 10^{-5} \text{ h}^{-1}$ (Paterson et al. 1990)
 $t_{1/2} > 1$ yr (O'Keefe et al. 1986)
 $t_{1/2} = 9.9\text{--}98$ yr (Geyer et al. 2000)
 degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000)
 $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
- Soil: $t_{1/2} = 10032\text{--}14160$ h, based on soil dieaway test data for two soils (Howard et al. 1991);
 $t_{1/2} \sim 1$ yr (Kearney et al. 1973; quoted, Quensen & Matsumura 1983);
 degradation $t_{1/2} = 10\text{--}12$ yr in soil (De Dimenico et al. 1980, Kimbrough et al. 1984);
 $t_{1/2} \sim 1$ yr if applied to surface on soil with 2,4-D (Nash & Beall 1980);
 $k \sim 8.0 \times 10^{-6} \text{ h}^{-1}$ (Mackay et al. 1985)
 $k \sim 1.1 \times 10^{-5} \text{ h}^{-1}$ (Paterson et al. 1990)
 $t_{1/2} = 10$ min during the day, photodegradation is a rapid process at the soil surface (Facchetti et al. 1986);
 $t_{1/2} \sim 10$ yr in soil if TCDD is on or near the surface and $t_{1/2} = 100$ yr if TCDD is buried at greater depth (Nauman & Schaum 1987)
 calculated $t_{1/2} = 10$ yr (Edujee 1987)
 $t_{1/2} = 10$ yr or longer (Boddington et al. 1990)
 $t_{1/2} = 365$ d for volatilization to atmosphere below surface soil (Jury et al. 1990)
 $t_{1/2} = 10$ yr (Geyer et al. 2000)
 degradation $t_{1/2} = 10\text{--}100$ yr in soils (estimated, Suzuki et al. 2000)
 $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000)
- Biota: $t_{1/2} = 31$ d, estimated half-life in rat (Rose et al. 1976; quoted, Birnbaum 1985);
 $t_{1/2} = 11$ d, estimated half-life in hamster (Olsen et al. 1980; quoted, Birnbaum 1985)
 $t_{1/2} = 30$ d, estimated half-life in guinea pig (Decad et al. 1981a; quoted, Birnbaum 1985)
 $t_{1/2} = 11\text{--}24$ d, estimated half-life in mouse (Gasiewicz et al. 1983; quoted, Birnbaum 1985)
 depuration $t_{1/2} = 58$ d, total body burden of ^{14}C -TCDD in whole rainbow trout (Branson et al. 1983, 1985)
 $t_{1/2} = 17\text{--}37$ d in mouse, $t_{1/2} = 31$ d in rat and $t_{1/2} = 30$ d in guinea pig (quoted, Van den Berg et al. 1985)
 elimination $t_{1/2} = 14.5$ d from fathead minnow (Adams et al. 1986)
 $t_{1/2} = 105$ d in whole body of rainbow trout (Kleeman et al. 1986);
 $t_{1/2} = 300\text{--}325$ d in carp (Kuehl et al. 1986)
 biological $t_{1/2} = 58$ d for rainbow trout (Niimi & Oliver 1986)
 $t_{1/2} = 5.8$ yr in human (estimated, Poiger & Schlatter 1986)
 $t_{1/2} > 336$ d for carps in Lake Superior (Kuehl et al. 1987)
 $t_{1/2} = 6.7$ yr in human (estimated, Kissel & Robarge 1988)
 elimination $t_{1/2} = 15\text{--}48$ d from rainbow trout for exposures of different concn (Mehrle et al. 1988)
 $t_{1/2} = 7.1$ yr in human (estimated, Pirkle et al. 1989; quoted, Webster & Connett 1991)
 $t_{1/2} = 5\text{--}8$ yr for human, $t_{1/2} = 17.4\text{--}31$ d for rats, $t_{1/2} = 9.6\text{--}24.4$ d for mice, $t_{1/2} = 22\text{--}93.7$ d for guinea pigs,
 $t_{1/2} = 12.0\text{--}150$ d for hamsters, $t_{1/2} = 1$ yr for monkeys (Boddington et al. 1990)
 $t_{1/2} = 40.3$ d for lactating cows (Olling et al. 1991)
 $t_{1/2} = 5\text{--}10$ yr assumed half-life for human (Schecter & Ryan 1991)
 elimination $t_{1/2} = 35\text{--}37$ d from lake trout sac fry (Walker et al. 1991)
 $t_{1/2} = 4.4$ yr for a 70 kg non-lactating "reference" human (Webster & Connett 1991)
 $t_{1/2} < 0.5$ d for metabolic inhibitor PBO treated gold fish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993)
 elimination $t_{1/2} = 45$ d from soft-shell clam (Brown et al. 1994)
 biological $t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994)
 reported $t_{1/2} = 8\text{--}24.4$ d for mice, $t_{1/2} = 30.2$ and 93.7 d for guinea pigs, $t_{1/2} = 20\text{--}28.9$ d for rats and $t_{1/2} = 365\text{--}3470$ d for humans (Miniero et al. 2001).
 depuration $t_{1/2} = 28$ d for newly contaminated oysters, and $t_{1/2} = 35$ d for chronically contaminated oysters (Gardinali et al. 2004)

TABLE 8.1.1.16.1
Reported vapor pressures of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin at various temperatures

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Schroy et al. 1985a		Schroy et al. 1985b		Webster et al. 1985		Rordorf 1987, 1989	
gas saturation		gas saturation		gas saturation-LSC		gas saturation-GC/ECD	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30.1	4.61×10^{-7}	30	4.67×10^{-7}	20	8.71×10^{-6}	25	2.0×10^{-7}
30.2	5.19×10^{-7}	54.6	1.83×10^{-5}	50	1.12×10^{-5}	50	9.5×10^{-6}
30.3	8.73×10^{-7}	62	4.97×10^{-5}	100	1.72×10^{-5}	75	2.6×10^{-4}
54.6	2.06×10^{-5}	71	1.59×10^{-4}			100	4.6×10^{-3}
55	1.37×10^{-5}					125	5.7×10^{-2}
55.2	1.94×10^{-5}	Antoine eq. for 10–305 °C					
61.9	3.71×10^{-5}	eq. 2	P/mmHg				$\Delta H_v/(kJ\ mol^{-1}) = 79.9$
62	4.58×10^{-5}	A	12.89784				$\Delta H_{subl}(kJ\ mol^{-1}) = 124.001$
70.9	1.79×10^{-4}	B	6477.132				$\Delta H_{fus}/(kJ\ mol^{-1}) = 39.9$
71	1.58×10^{-4}	C	273.15				$\Delta S_{fus}/(J\ mol^{-1}\ K^{-1}) = 69$
71.1	1.59×10^{-4}						
		Antoine eq. for 305–420 °C					
eq. 1	P/Pa	eq. 2	P/mmHg				
A	34.570834	A	8.78307				
B	14903.438	B	4098.173				
		C	273.15				

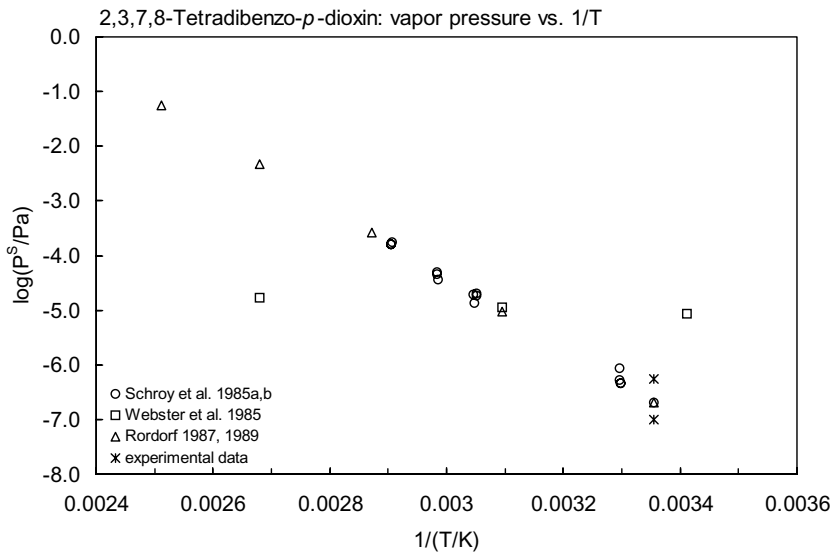


FIGURE 8.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.

TABLE 8.1.1.16.2
Reported octanol-air partition coefficients of 2,3,7,8-
tetrachlorodibenzo-*p*-dioxin at various temperatures

Harner et al. 2000	
generator column-GC/ECD	
$t/^{\circ}\text{C}$	K_{OA}
20	10.318
40	9.283
50	8.778
25	10.05
$\log K_{\text{OA}} = a + b/(T/\text{K})$	
a	-6.19
b	4840
enthalpy of phase change	
$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 92.60$	

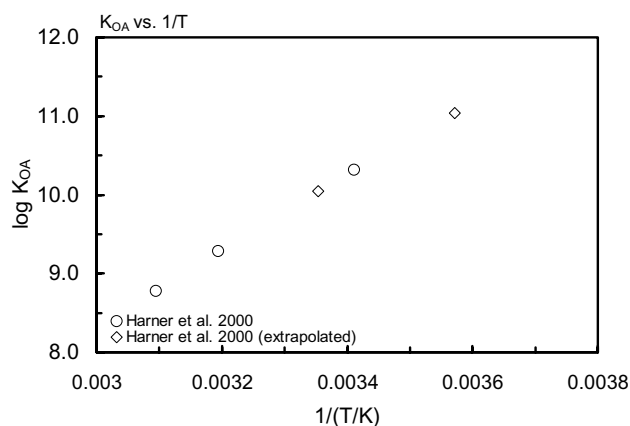
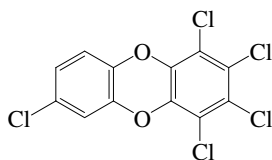


FIGURE 8.1.1.16.2 Logarithm of K_{OA} versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.

8.1.1.17 1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4,7-P₅CDD

Chemical Name: 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin

CAS Registry No: 39227-61-7

Molecular Formula: ClC₆H₃O₂C₆Cl₄

Molecular Weight: 356.416

Melting Point (°C):

195 (Lide 2003)

Boiling Point (°C):

464.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

197.74 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

92.8 (Rordorf 1987)

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

137.419 (Rordorf 1987)

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

42.4 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

26 (Friesen & Webster 1990)

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

90 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0215 (mp at 195°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

0.000118*; 0.0000855 (20°C, ¹⁴C-labelled, generator column-HPLC/LSC, measured range 20–40°C, calculated, Friesen et al. 1985)

0.0000955 (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, Webster et al. 1986)

1.23 × 10⁻⁴* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)

0.00428 (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)

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

8.80 × 10⁻⁸* (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.00 × 10⁻⁶ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

1.00 × 10⁻⁶ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

log (P/Pa) = 17.02207 – 7179.05/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

4.57 × 10⁻⁶ (supercooled liquid P_L, GC-RI correlation; Wang & Wong 2002)

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

0.264 (calculated-P/C, Shiu et al. 1988; quoted, Kaupp & McLachlan 1999)

0.224; 1.23 (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

0.691; 1.23 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

- 9.44, 9.62, 10.02; 9.39, 9.65, 10.05 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 9.40, 9.65 (HPLC-RT correlation, Sarna et al. 1984)
 9.48, 8.80; 9.40, 8.64 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 9.65, 7.44 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 6.60 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)
 7.53 (GC-RI correlation, Wang & Wong 2002)

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

Additional data at other temperatures designated * are compiled at the end of this section:

- 10.67*; 10.32 (generator column-GC; calculated, Harner et al. 2000)
 $\log K_{OA} = -7.65 + 5460/(T/K)$, temp range 30–50°C (Harner et al. 2000)
 10.42 (GC-retention time correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 3.26 (fathead minnow, steady-state, wet weight, Muir et al. 1985)
 2.50 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
 3.16, 2.91 (fathead minnow, rainbow trout, De Voogt et al. 1990;)
 3.50, 4.50 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 5.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

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

- 4.85, 4.60, 4.50 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986b)
 5.80, 5.67, 5.90 (20, 30, 40°C, humic acid from Manitoba peat bog, Webster et al. 1986b)
 6.38, 6.39, 6.46 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986b)
 5.02 (DOC, De Voogt et al. 1990)
 8.57 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

Photolysis: rate constant $k = 4.31 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) at 313 nm and calculated half-lives under conditions of variable sunlight intensity at 40°N latitude: $t_{1/2} = 18.29 \text{ d}$ in spring with rate constant $k = 0.466 \times 10^{-6} \text{ s}^{-1}$, $t_{1/2} = 15.16 \text{ d}$ in summer with $k = 0.562 \times 10^{-6} \text{ s}^{-1}$, $t_{1/2} = 28.59 \text{ d}$ in fall with $k = 0.298 \times 10^{-6} \text{ s}^{-1}$, $t_{1/2} = 52.37 \text{ d}$ in winter with $k = 0.163 \times 10^{-6} \text{ s}^{-1}$, and $t_{1/2} = 76.82 \text{ d}$ averaged over full year with rate constant $k = 0.111 \times 10^{-6} \text{ s}^{-1}$ (Choudhary & Webster 1985a, 1986);

$k = 4.3115 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (3:3 v/v) at 313 nm (Choudhary & Webster 1985b);

photolysis $k = 4.31 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 45.86 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 4.03 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 18 \text{ d}$ in spring, $k = 4.86 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 15 \text{ d}$ in summer, $k = 2.58 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 29 \text{ d}$ in fall, $k = 1.41 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 52 \text{ d}$ in winter (Choudhary & Webster 1989);

$k = 0.74 \text{ d}^{-1}$ under mid-summer sunlight at 50°N latitude in filtered-sterilized natural water and $k = 0.058 \text{ d}^{-1}$ in (2:3, v/v) distilled water-acetonitrile (Friesen et al. 1990);

photolytic $t_{1/2} = 38 \text{ h}$ in fly-ash extract (Tysklind & Rappe 1991);

$t_{1/2} = 92 \text{ h}$ for photodegradation in a rotary photoreactor adsorbed to clean silica gel by filtered <290 nm of light (Koester & Hites 1992).

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

$k_{OH}(\text{calc}) = (12 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (6.5 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.1\text{--}2.4 \text{ d}$ based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.7 - 3.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 4.0\text{--}8.5 \text{ d}$ for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation: biotransformation rate constant $k = 0.014 \text{ d}^{-1}$ for rainbow trout (Sijm et al. 1990).

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

$k_1 = 285 \text{ d}^{-1}$; $k_2 = 0.22 \text{ d}^{-1}$ (fathead minnow, flow-through system, Muir et al. 1985)

$k_1 = 204 \text{ d}^{-1}$; $k_2 = 0.28 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_2 = 2.5 \times 10^{-2}$, $3.9 \times 10^{-2} \text{ d}^{-1}$ (rainbow trout for 2 to 21 d exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1990)

$k_1 = 509$, $162 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1$, $> 1.5 \text{ d}^{-1}$ (goldfish after 120-h exposure for metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 169 \text{ L kg}^{-1} \text{ d}^{-1}$, $251 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P₃CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime of 1.1–2.4 d calculated for the gas-phase with OH radicals using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, (Atkinson 1991);

photodegradation $t_{1/2} = 92 \text{ h}$ in a rotary photo-reactor adsorbed to clean silica gel by filtered $\lambda < 290 \text{ nm}$ of light (Koester & Hites 1992);

calculated tropospheric lifetime of 4.0–8.5 d for penta-chlorinated dioxin for the gas-phase reaction with OH radical at room temp. (Kwok et al. 1995);

suggested $t_{1/2} = 200 \text{ h}$ at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000).

Surface water: under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile solution (4:6, v/v): $t_{1/2} = 18.29 \text{ d}$ in spring, $t_{1/2} = 15.16 \text{ d}$ in summer, $t_{1/2} = 28.6 \text{ d}$ in fall, $t_{1/2} = 52.37 \text{ d}$ in winter, and $t_{1/2} = 76.82 \text{ d}$ averaged over full year (Choudhary & Webster 1985a, 1986);

photolysis $t_{1/2} = 45.86 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct phototransformation half-lives near water bodies at 40°N latitude: $t_{1/2} = 18.4 \text{ d}$ in spring, $t_{1/2} = 15 \text{ d}$ in summer, $t_{1/2} = 29 \text{ d}$ in fall and $t_{1/2} = 52 \text{ d}$ in winter (Choudhary & Webster 1989);

$t_{1/2} = 27 \text{ d}$ in sunlit surface water and $t_{1/2} = 0.94 \text{ d}$ in surface water of actual pond (Friesen et al. 1990).

Groundwater:

Sediment: degradation half-lives in sediment 20–200 yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation half-lives in soil 10–100 yr (estimated, Suzuki et al. 2000).

Biota: $t_{1/2} = 3.1 \text{ d}$ in fathead minnow (Adams et al. 1986);

$t_{1/2} = 2 \text{ d}$ in whole body of rainbow trout (Muir & Yarechewski 1988);

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

TABLE 8.1.1.17.1

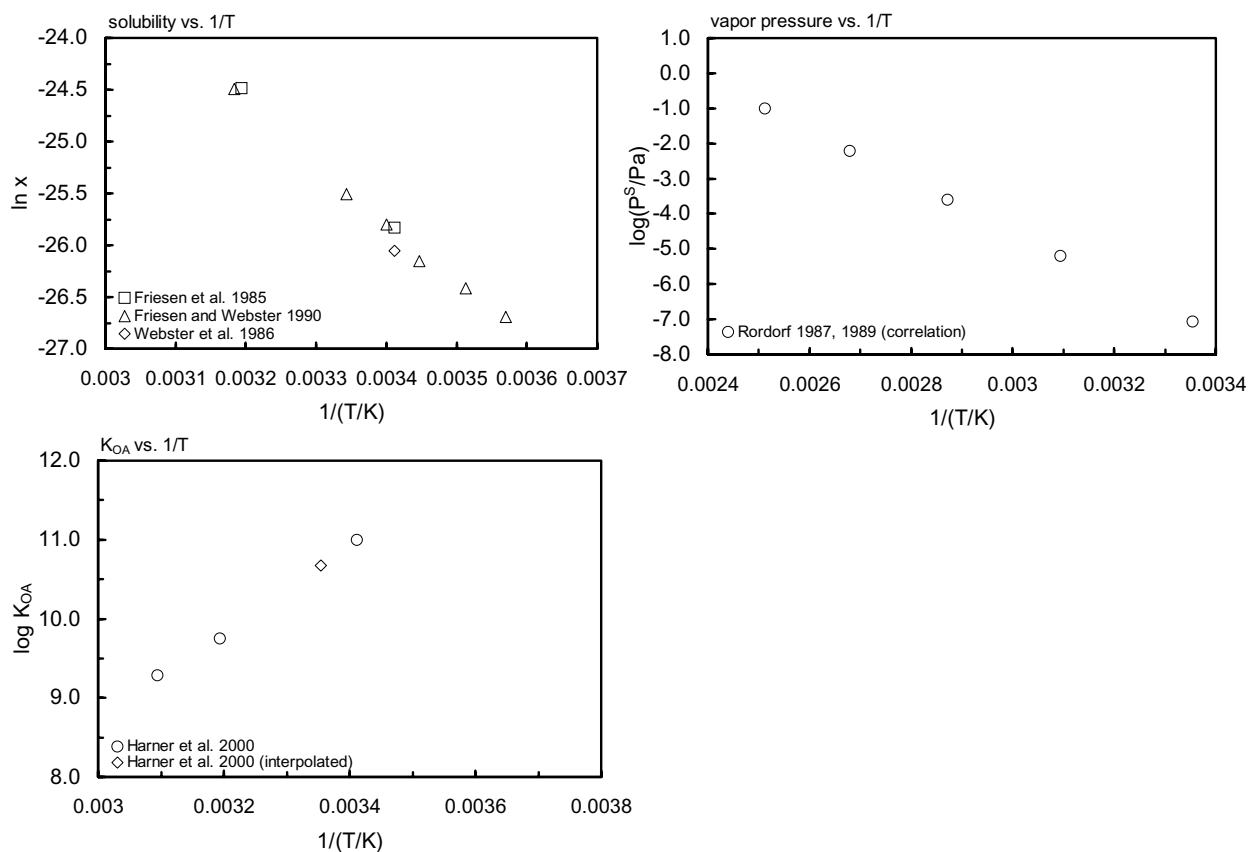
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin at various temperatures

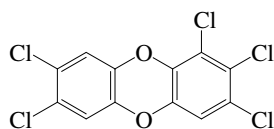
Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	log K_{OA}
20	1.20×10^{-4}	7	5.05×10^{-5}	25	8.8×10^{-8}	20	10.996
40	3.17×10^{-4}	11.5	6.70×10^{-5}	50	6.4×10^{-6}	40	9.751
		17	8.70×10^{-5}	75	2.5×10^{-4}	50	9.282
		21	1.24×10^{-4}	100	6.1×10^{-3}	25	10.67
		26	1.65×10^{-4}	125	9.8×10^{-2}		
		41	4.56×10^{-4}				
						log $K_{OA} = a + b/(T/K)$	

(Continued)

TABLE 8.1.1.17.1 (Continued)

Aqueous solubility				Vapor pressure		log K _{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K _{OA}
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 47.5$ 7–41 °C		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 92.8$ $\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 131.42$ $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 42.4$ $\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 90$		a -7.65 b 5460 enthalpy of phase change $\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 104.0$	

FIGURE 8.1.1.17.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin.

8.1.1.18 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,7,8-P₅CDD

Chemical Name: 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin

CAS Registry No: 40321-76-4

Molecular Formula: Cl₂C₆H₂O₂C₆HCl₃

Molecular Weight: 356.416

Melting Point (°C):

Boiling Point (°C):

464.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

195.74 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.7 (Rordorf 1987)

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

134.062 (Rordorf 1987)

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

42.4 (Rordorf 1987)

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

83 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

0.000722 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):

9.82×10^{-5} (calculated-QSAR, Fielder & Schramm 1990)

2.77×10^{-3} (supercooled liquid S_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(\text{mol/L})] = 0.445 - 2232/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

4.0×10^{-3} ; 2.77×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

5.80×10^{-8} * (calculated, Rordorf 1985a,b, 1987,1989; quoted, Kaupp & McLachlan 1999)

1.20×10^{-5} (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

1.71×10^{-4} ; 1.23×10^{-7} (supercooled liquid P_L; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.72 - 5850/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 8.38 - 3321/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

4.17×10^{-6} ; 1.20×10^{-5} (supercooled liquid P_L; GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

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

$\log (H/(\text{Pa m}^3/\text{mol})) = 7.94 - 1089/(T/K)$ (Passivirta et al. 1999)

0.661; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

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

7.27 (estimated-solubility S_L and regression eq. using lit. K_{ow} values, Passivirta et al. 1999)

- 7.215 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 7.55; 7.50 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
 6.78, 6.84, 6.49, 6.87 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 10.57*; 10.44 (generator column-GC; calculated, Harner et al. 2000)
 11.63 (7°C, GC-retention time correlation, Harner et al. 2000)
 $\log K_{OA} = -8.02 + 5540/(T/K)$; temp range 30–50°C (generator column-GC/ECD, Harner et al. 2000)
 10.46 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 3.20 (guppy, exposed to fly ash extract, Opperhuizen et al. 1986)
 3.93; 4.31 (goldfish: PBO treated; control, 120-h exposure, Sijm et al. 1993)
 5.27 (guppies, 21-d exposure, system-I absence of sediment, Loonen et al. 1994b)
 4.98 (guppies, 21-d exposure, system-II with sediment, Loonen et al. 1984b)
 5.34 (calculated-SOFA model, Govers & Krop 1998)

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

- 5.91 (calculated-QSAR, Fiedler & Schramm 1990)
 6.80 (Baltic sea particulate field samples, concentration distribution-GC/MS, Broman et al. 1991)
 8.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

Photolysis: solution photolysis $t_{1/2} = 456$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 52.8$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984);

photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with $t_{1/2} = 33.6$ h for native congener and $t_{1/2} = 16.7$ h for ^{13}C -labeled congener in tetradecane solution (Tysklind & Rappe 1991);

$t_{1/2} = 57.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

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

$k_{OH}(\text{calc}) = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (6.5 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.1\text{--}2.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.7 - 3.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 4.0\text{--}8.5$ d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 700 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.090 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1986)

$k_1 = 127, 695 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.02, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure, Sijm et al. 1993)

$k_1 = 169 \text{ L kg}^{-1} \text{ d}^{-1}$, $251 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_3CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 952 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.030 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0051 \text{ d}^{-1}$ with $t_{1/2} = 50$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: for a penta-chlorinated dioxin, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime $\tau = 1.1\text{--}2.4$ d for the gas phase with OH radical (Atkinson 1991);

calculated tropospheric lifetime $\tau = 4.0\text{--}8.5$ d for reaction with OH radical (Kwok et al. 1995);
 $t_{1/2} = 360$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: $t_{1/2} = 7200$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Groundwater:
Sediment: $t_{1/2} = 1000000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000).
Soil: $t_{1/2} = 1,000,000$ h at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000);
degradation $t_{1/2} = 10\text{--}100$ yr in soil (estimated, Suzuki et al. 2000).
Biota: half-lives in gold fish: $t_{1/2} = 32$ d for PBO treated and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993);
 $t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.18.1
Reported vapor pressures and octanol-air partition coefficients of 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin at various temperatures

Vapor pressure		log K_{OA}	
Rordorf 1987, 1989		Harner et al. 2000	
vapor pressure correlation		generator column-GC/ECD	
t/°C	P/Pa	t/°C	log K_{OA}
25	5.8×10^{-8}	20	10.867
50	3.8×10^{-6}	40	9.755
75	1.4×10^{-4}	50	9.083
100	3.0×10^{-3}	25	10.57
125	4.6×10^{-2}		
$\Delta H_v/(\text{kJ mol}^{-1}) = 88.7$		$\log K_{OA} = a + b/(T/K)$	
$\Delta H_{sub}/(\text{kJ mol}^{-1}) = 138.062$		a	-8.02
$\Delta H_{fus}/(\text{kJ mol}^{-1}) = 42.4$		b	5540
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 106$	
		for GC-RT correlation	

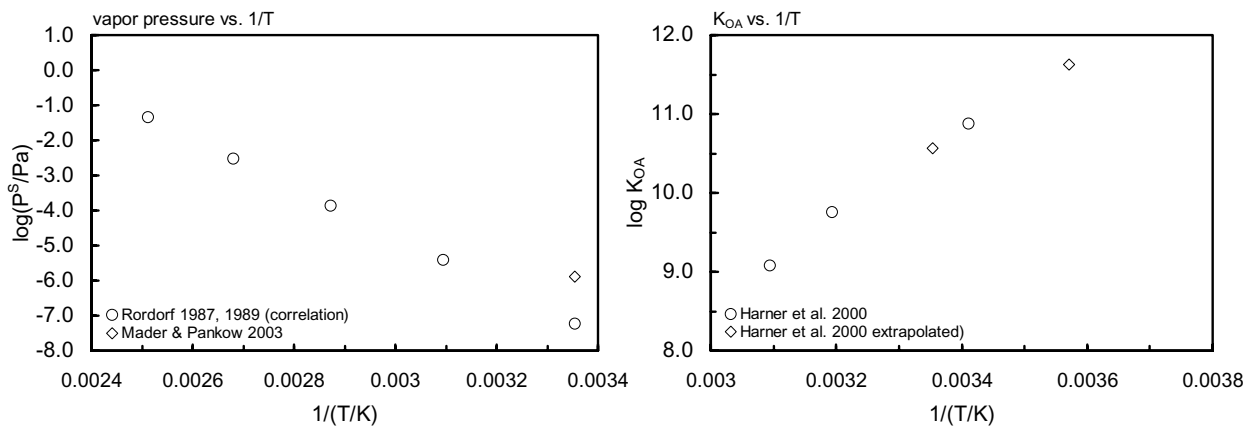
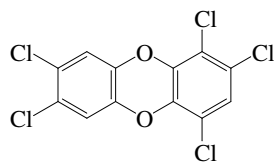


FIGURE 8.1.1.18.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin.

8.1.1.19 1,2,4,7,8-Pentachlorodibenzo-*p*-dioxin

Common Name: 1,2,4,7,8-Pentachlorodibenzo-*p*-dioxin

Synonym: 1,2,4,7,8-P₅CDD

Chemical Name: 1,2,4,7,8-pentachlorodibenzo-*p*-dioxin

CAS Registry No: 58802-08-7

Molecular Formula: Cl₅C₆H₂O₂C₆HCl₃

Molecular Weight: 356.416

Melting Point (°C):

206 (Rordorf 1987)

Boiling Point (°C):

464.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

199.91 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.8 (Rordorf 1987)

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

136.636 (Rordorf 1987)

125.3 (Li et al. 2004)

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

42.4 (Rordorf 1987)

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

88 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0168 (mp at 206°C)

Water Solubility (g/m³ or mg/L at 25°C):

9.82 × 10⁻⁵ (calculated-QSAR, Fielder & Schramm 1990)

4.92 × 10⁻³ (supercooled liquid S_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

5.39 × 10⁻³; 4.92 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):

7.80 × 10⁻⁸, 5.6 × 10⁻⁶, 2.1 × 10⁻⁴, 5.1 × 10⁻³, 8.0 × 10⁻² (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.58 × 10⁻⁵ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)

6.026 × 10⁻⁶; 1.58 × 10⁻⁵ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

ln (P/Pa) = 38.743 – 16431/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

ln (P/Pa) = (36.472 ± 0.679) – (15073 ± 282)/(T/K); temp range 403–428 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol):

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

7.41; 1.096 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

8.41 (calculated-QSAR, Fiedler & Schramm 1990)

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

7.46; 7.36 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.20; 6.71, 6.78, 6.55, 6.87 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

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

Bioconcentration Factor, $\log BCF$:

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

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

5.91 (calculated-QSAR, Fiedler & Schramm 1990)

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

Volatilization:

Photolysis: $t_{1/2} = 81.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

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

$k_{OH}(\text{calc}) = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (6.5 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime of 1.1 – 2.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.7 - 3.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 4.0–8.5 d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 61, 164 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.21, > 1.9 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure, Sijm et al. 1993)

$k_1 = 169 \text{ L kg}^{-1} \text{ d}^{-1}$, $251 \text{ L kg}^{-1} \text{ d}^{-1}$ (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: tropospheric lifetime $\tau = 1.1\text{--}2.4$ d calculated for a penta-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

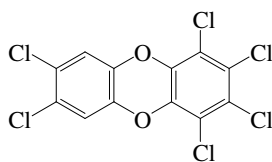
Surface water:

Groundwater:

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

Soil: degradation $t_{1/2} = 10\text{--}100$ yr in soil (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 3.3$ d for PBO treated and $t_{1/2} > 1.9$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.20 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4,7,8-H₆CDD

Chemical Name: 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin

CAS Registry No: 39227-26-8

Molecular Formula: Cl₂C₆H₂O₂C₆Cl₄

Molecular Weight: 390.861

Melting Point (°C):

273–275 (Pohland & Yang 1972; Rordorf 1987,1989; Delle Site 1997)

Boiling Point (°C):

487.7 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

206.96 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

89.1 (Rordorf 1987)

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

140.782 (Rordorf 1987)

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

48.1 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

30.21 (Friesen & Webster 1990)

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

88 (Rordorf 1987, 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F: 0.00369 (assuming ΔS_{fus} = 56 J/mol K and mp at 273°C)

0.00352 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)

0.000148 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4.40 × 10⁻⁶* (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)

5.70 × 10⁻⁶ (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, Webster et al. 1986b)

4.89 × 10⁻⁶* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)

log [S_L/(mol/L)] = 0.235 B 2515/(T/K) (supercooled liquid, Passivirta et al. 1999)

1.15 × 10⁻³ (supercooled liquid S_L; GC-RI correlation, Wang & Wong 2002)

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

5.10 × 10⁻⁹* (calculated-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

3.20 × 10⁻⁷ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

3.96 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)

5.43 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)

1.00 × 10⁻⁸ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

1.45 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

1.36 × 10⁻⁹, 1.87 × 10⁻⁹ (solid P_S, calculated from reported P_L, Delle Site 1997)

3.19 × 10⁻⁶ (corrected supercooled liquid P_L, Eitzer & Hites 1998)

5.20 × 10⁻⁵; 7.70 × 10⁻⁹ (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.97 - 6282/(T/\text{K})$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 8.37 - 3769/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P/\text{Pa}) = 15.65106 - 7087.08/(T/\text{K})$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 3.72×10^{-5} (supercooled liquid P_L , Harner et al. 2000)
 8.91×10^{-7} (supercooled liquid P_L ; GC-RI correlation; Wang & Wong 2002)

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

0.452 (calculated-P/C, Shiu et al. 1988; quoted, Kaupp & McLachlan 1999)
 0.631; 1.45 (quoted lit., calculated-SOFA model, Govers & Krop 1998)
 $\log (H/(\text{Pa m}^3/\text{mol})) = 8.14 - 1254/(T/\text{K})$ (Passivirta et al. 1999)
 0.427; 1.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

10.36, 10.39, 10.89; 10.22, 10.44, 10.89 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 10.40, 9.65; 10.22, 9.19 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 10.44, 7.79 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 7.80 (selected, Shiu et al. 1988)
 8.0 (calculated-QSAR, Fiedler & Schramm 1990)
 7.30 (calculated, Broman et al. 1991)
 9.53 (HPLC-RT correlation, Chessells et al. 1991)
 9.13 (calculated-fragment const., Chessells et al. 1991)
 10.22 (quoted, Hansch et al. 1995)
 7.94 (calculated-SOFA model, Govers & Krop 1998)
 7.90 (estimated-solubility S_L and regression eq. using lit. K_{ow} values, Passivirta et al. 1999)
 7.628 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 7.94; 7.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
 7.80; 7.12, 7.12, 7.25, 7.30 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

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

Additional data at other temperatures designated * are compiled at the end of this section:

11.50 (calculated- K_{ow}/K_{Aw} , Wania & Mackay 1996)
 11.17 (calculated, Finizio et al. 1997)
 11.11*; 10.88 (generator column-GC; calculated, Harner et al. 2000)
 12.20 (7°C, GC-retention time correlation, Harner et al. 2000)
 $\log K_{OA} = -6.20 + 5160/(T/\text{K})$; temp range 30–50°C (generator column-GC/ECD, Harner et al. 2000)
 10.95 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

3.73, 4.00 (rainbow trout, fathead minnow, steady-state, wet weight, Muir et al. 1985)
 4.00, 5.00 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 3.41, 3.76 (fathead minnow, quoted, Opperhuizen & Sijm 1990)
 3.45, 3.23 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
 3.45, 4.87 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
 5.01; 4.65 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 5.01; 5.01; 5.14 (guppy, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 5.01; 5.07 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 5.90, 5.98 (fish muscle $\log BCF_L$ calculated from water, calculated from sediment, Wu et al. 2001)

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

5.41, 5.31, 5.13 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986)
 6.02, 6.15, 5.95 (20, 30, 40°C, humic acid from Manitoba peat bog, Webster et al. 1986)
 6.32, 6.27, 6.15 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986b)
 5.02 (DOC, De Voogt et al. 1990)
 7.10 (Baltic Sea particulate field samples, concentration distribution-GC/MS, Broman et al. 1991)

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

Volatilization:

Photolysis:

$k(\text{calc}) = 1.06 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 7.57 \text{ d}$ in spring, $k = 1.280 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 6.27 \text{ d}$ in summer, $k = 0.676 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 11.87 \text{ d}$ in autumn, $k = 0.37 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 21.57 \text{ d}$ in winter and the averaged $k = 0.252 \times 10^{-6} \text{ s}^{-1}$ over full year with $t_{1/2} = 31.85 \text{ d}$, under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile (4:6 v/v) solution (Choudhary & Webster 1985a,c, 1986)

$k = 7.86 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhary & Webster 1985b)

$k = 7.86 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 24.5 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons:

$k = 9.16 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 7.6 \text{ d}$ in spring, $k = 11.06 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 6.3 \text{ d}$ in summer, $k = 5.84 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 12.0 \text{ d}$ in fall, $k = 3.21 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 22.0 \text{ d}$ in winter (Choudhary & Webster 1989)

$k = 0.28 \text{ d}^{-1}$ in natural water and $k = 0.019 \text{ d}^{-1}$ in distilled water-acetonitrile (Friesen et al. 1990)

photolytic $t_{1/2}(\text{calc}) = 38 \text{ h}$ in the fly ash extract in tetradecane (Tysklind & Rappe 1991)

photodegradation $t_{1/2} = 140 \text{ h}$ in a rotary photoreactor absorbed to silica gel by filtered $< 290 \text{ nm}$ of light (Koester & Hites 1992)

$t_{1/2} = 91.8 \text{ h}$ on spruce needles surface under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{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 PCDD is $5.02 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (4.6 - 10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.5\text{--}3.4 \text{ d}$ based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 102 \text{ d}^{-1}$; $k_2 = 0.046 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_1 = 112 \text{ d}^{-1}$; $k_2 = 0.030 \text{ d}^{-1}$ (fathead minnow, Muir et al. 1985)

$k_2 = 0.030 \text{ d}^{-1}$ (fathead minnow, Muir et al. 1985)

$k_2 = 0.015 \text{ d}^{-1}$ (rainbow trout, Muir & Yarechewski 1988)

$k_2 = 0.0066 \text{ d}^{-1}$ (fathead minnow, Muir & Yarechewski 1988)

$k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}$, $299 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.29$, $> 0.02 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1993)

$k_1 = 868 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.065 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0105 \text{ d}^{-1}$ with $t_{1/2} = 29 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: estimated reaction rate constant, $k = 0.005 \text{ h}^{-1}$ (Paterson et al. 1990);

tropospheric lifetime $\tau = 1.5\text{--}3.4 \text{ d}$ for a hexa-chlorinated dioxin reaction with the OH radicals using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, (Atkinson 1991);

photodegradation $t_{1/2} = 140 \text{ h}$ in a rotary photoreactor adsorbed to clean silica gel by filtered $\lambda < 290 \text{ nm}$ of light, (Koester & Hites 1992);

suggested $t_{1/2} = 740 \text{ h}$ at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000).

Surface water: under conditions of variable sunlight intensity at 40°N latitude: $t_{1/2} = 7.57 \text{ d}$ in spring, $t_{1/2} = 6.27 \text{ d}$ in summer, $t_{1/2} = 11.87 \text{ d}$ in fall, $t_{1/2} = 21.57 \text{ d}$ in winter, and $t_{1/2} = 76.8 \text{ d}$ averaged over full year (Choudhary & Webster 1985a, 1986);

photolysis $t_{1/2} = 24.5 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct phototransformation half-lives near water bodies at 40°N latitude: 7.6 d in spring, 6.3 d in summer, 12.0 d in fall and 22.0 d in winter (Choudhary & Webster 1989);

$t_{1/2} = 81 \text{ d}$ in sunlit surface water and $t_{1/2} = 2.5 \text{ d}$ in surface water of actual pond (Friesen et al. 1990);

estimated reaction rate constant, $k = 0.002 \text{ h}^{-1}$ (Paterson et al. 1990);

suggested $t_{1/2} = 14800 \text{ h}$ at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: estimated reaction rate constant $k = 4.0 \times 10^{-6} \text{ h}^{-1}$ (Paterson et al. 1990);

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

suggested $t_{1/2} = 2400000 \text{ h}$ at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: estimated reaction rate constant $k = 2.8 \times 10^{-6} \text{ h}^{-1}$ (Paterson et al. 1990);

degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ in soil for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 2400000 \text{ h}$ at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} = 43 \text{ d}$ in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);

half-lives in gold fish: $t_{1/2} = 2.4 \text{ d}$ for PBO treated and $t_{1/2} = 40 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 29 \text{ d}$ in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.20.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	log K_{OA}
20	4.40×10^{-6}	7	2.31×10^{-6}	25	5.1×10^{-9}	20	11.403
40	1.90×10^{-5}	11.5	3.12×10^{-6}	50	4.1×10^{-7}	40	10.297
		17	4.18×10^{-6}	75	1.8×10^{-5}	50	9.762
		21	4.89×10^{-6}	100	4.6×10^{-4}	25	11.11
		26	7.90×10^{-6}	125	8.0×10^{-3}		
		41	1.90×10^{-5}				
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 45.5$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 89.1$		log $K_{OA} = a + b/(T/K)$	
		7–41 $^\circ\text{C}$		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 140.78$		a	–6.20
				$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 48.1$		b	5160
				$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 88$		enthalpy of phase change	
						$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 98.70$	

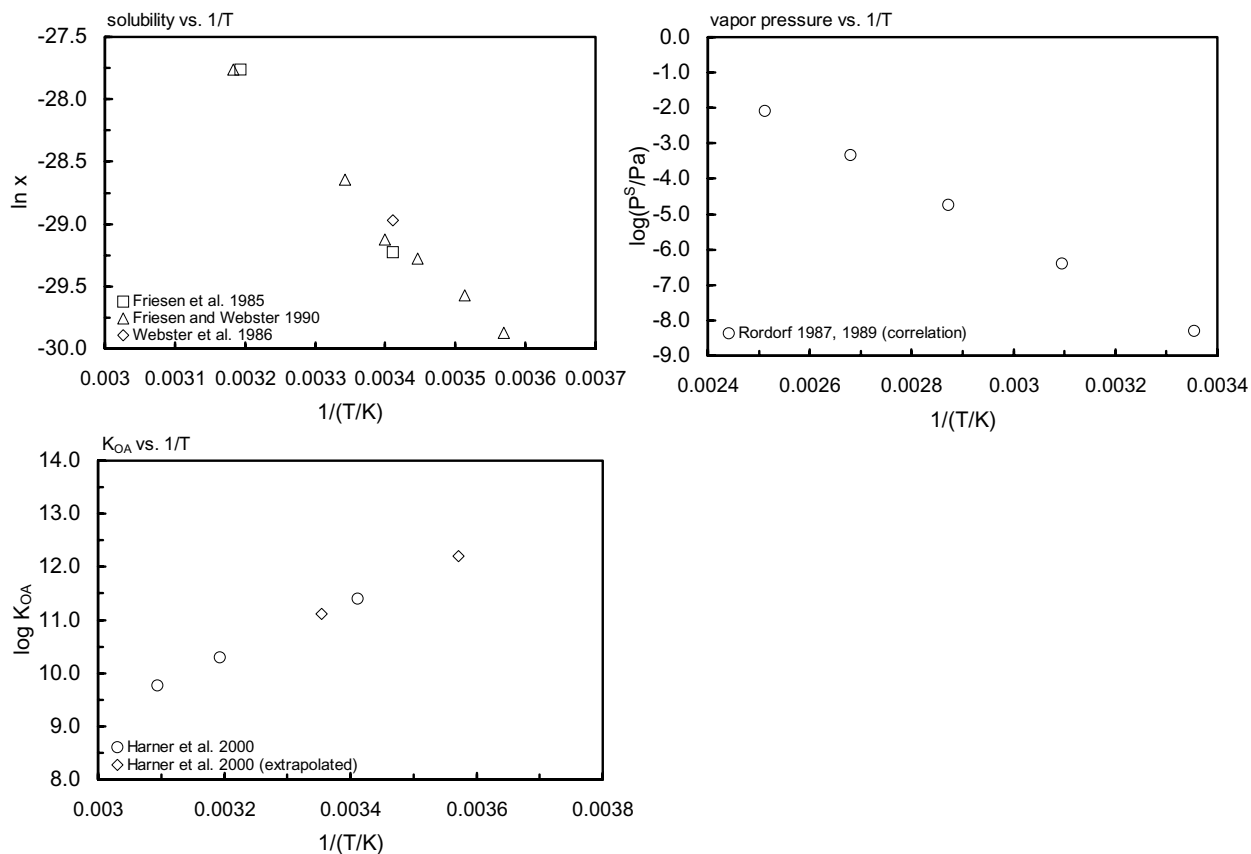
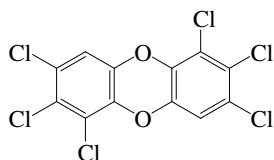


FIGURE 8.1.1.20.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin.

8.1.1.21 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,6,7,8-H₆CDD

Chemical Name: 1,2,3,6,7,8-hexachlorodibenzo-*p*-dioxin

CAS Registry No: 57653-85-7

Molecular Formula: Cl₃C₆HO₂C₆HCl₃

Molecular Weight: 390.861

Melting Point (°C):

285 (Lide 2003)

Boiling Point (°C):

487.7 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

207.16 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.1 (Rordorf 1987)

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

139.975 (Rordorf 1987)

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

48.1 (Rordorf 1987)

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

86 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C, F: 0.00281 (assuming ΔS_{fus} = 56 J/mol K and mp at 185°C)

0.000167 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):

8.75×10^{-4} (calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(\text{mol/L})] = 0.125 - 2515/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.10×10^{-3} , 8.75×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):

4.80×10^{-9} , 3.80×10^{-7} , 1.60×10^{-5} , 4.0×10^{-4} , 6.9×10^{-3} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

3.31×10^{-6} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)

5.20×10^{-5} ; 8.69×10^{-9} (supercooled liquid P_L; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.96 - 6363/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 8.47 - 3751/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

8.51×10^{-7} , 3.31×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

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

$\log [H/(\text{Pa m}^3/\text{mol})] = 8.35 - 1236/(T/K)$ (Passivirta et al. 1999)

0.417; 1.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

9.13 (calculated-QSAR, Fiedler & Schramm 1990)

7.80 (calculated, Broman et al. 1991)

- 7.98 (calculated-SOFA model, Govers & Krop 1998)
- 7.96 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 7.639 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.94; 7.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
- 7.58 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

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

- 12.22 (7°C, GC-retention time correlation, Harner et al. 2000)
- 10.97 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 3.41, 4.61 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
- 4.94; 4.70 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
- 4.94; 5.05; 5.24 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
- 5.98 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
- 5.56 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)

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

- 6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
- 7.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 9.42 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

- Photolysis: solution photolysis $t_{1/2} = 379$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 44100$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984);
- photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with $t_{1/2} = 17.3$ h for native congener and $t_{1/2} = 14.2$ h for ^{13}C -labeled congener in tetradecane solution (Tysklind & Rappe 1991);
- $t_{1/2} = 76.2$ h on spruce needle surface under sunlight irradiation (Niu et al. 2003).

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

$k_{OH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (4.6 - 10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.5\text{--}3.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 432 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 120-h exposure, control fish, Sijm et al. 1993)

$k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}$, $299 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.23, < 0.1 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 844 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.050 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0075 \text{ d}^{-1}$ with $t_{1/2} = 60$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991);

$t_{1/2} = 740$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 14800$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20$ –200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 550000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

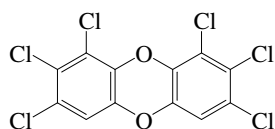
Soil: degradation $t_{1/2} = 10$ –100 yr in soil for all homologues (estimated, Suzuki et al. 2000);

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

Biota: 43 d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);

$t_{1/2} = 3.0$ d for PBO treated gold fish, $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 40$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

8.1.1.22 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,7,8,9-H₆CDD OR 2,3,4,6,7,8-H₆CDD

Chemical Name: 1,2,3,7,8,9-hexachlorodibenzo-*p*-dioxin

CAS Registry No: 19408-74-3

Molecular Formula: Cl₃C₆HO₂C₆HCl₃

Molecular Weight: 390.861

Melting Point (°C):

243–244 (Rordorf 1987)

Boiling Point (°C):

487.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

207.16 (calculated-liquid density, Govers et al. 1990)

210.16 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.7 (Rordorf 1987)

103.9 (GC-RI correlation, Govers et al. 1995)

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

142.922 (Rordorf 1987)

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

48.1 (Rordorf 1987)

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

93 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C, F:

0.00027 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):

6.34×10^{-4} (calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(\text{mol/L})] = 0.491 - 2515/(T/K)$ (liquid, Passivirta et al. 1999)

1.10×10^{-3} , 6.34×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

6.50×10^{-9} , 5.60×10^{-7} , 2.60×10^{-5} , 7.00×10^{-4} , 1.30×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.38×10^{-6} (calculated-SOFA model, Govers & Krop 1998)

4.51×10^{-5} ; 1.22×10^{-8} (supercooled liquid P_L; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.93 - 6211/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 8.07 - 3699/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

8.51×10^{-7} , 1.38×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

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

$\log [H/(\text{Pa m}^3/\text{mol})] = 7.58 - 1184/(T/K)$ (Passivirta et al. 1999)

0.417; 0.832 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

6.90 (calculated, Broman et al. 1991)

- 8.02 (calculated-SOFA model, Govers & Krop 1998)
- 7.76 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 7.61 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.95; 8.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
- 7.58 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

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

- 12.26 (7°C, GC-retention time correlation, Harner et al. 2000)
- 11.01 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 2.95 (guppy exposed to fly ash extract, Opperhuizen et al. 1986)
- 3.50, 4.02 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
- 4.93; 4.34 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
- 4.99; 4.94; 5.02 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from nonlinear regression analysis, Loonen et al. 1994b)
- 5.18 (calculated-SOFA model, Govers & Krop 1998)
- 5.29 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)

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

- 6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
- 6.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 9.45 (calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

Photolysis: photolytic $t_{1/2} = 5.4$ h when exposed to sunlight in hexane solution (Doobs & Grant 1979)

photolytic degradation $t_{1/2} = 17.1$ h in extract from fly ash exposed to UV light from a distance of 20 cm in tetradecane solution (Tysklind & Rappe 1991)

$t_{1/2} = 92.4$ h on spruce needle surface under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{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 PCDD) is $5.02 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{OH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (4.6 - 10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime of 1.5 – 3.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 200 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.210 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1986)

$k_1 = 48, 433 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.44, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}$, $299 \text{ L kg}^{-1} \text{ d}^{-1}$ (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)

$k_1 = 687 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.074 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0057 \text{ d}^{-1}$ with $t_{1/2} = 52 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} , the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991)

$t_{1/2} = 740$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_{1/2} = 14800$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20$ –200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);

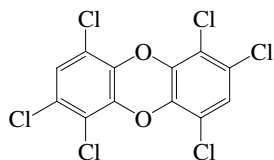
$t_{1/2} = 2400000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 10$ –100 yr in soil for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 2400\,000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: half-lives in gold fish: 1.6 d for PBO treated and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 52$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

8.1.1.23 1,2,4,6,7,9-Hexachlorodibenzo-*p*-dioxin

Common Name: 1,2,4,6,7,9-Hexachlorodibenzo-*p*-dioxin

Synonym: 1,2,4,6,7,9-H₆CDD

Chemical Name: 1,2,4,6,7,9-hexachlorodibenzo-*p*-dioxin

CAS Registry No: 39227-62-8

Molecular Formula: Cl₃C₆HO₂C₆HCl₃

Molecular Weight: 390.861

Melting Point (°C):

238–240 (Pohland & Yang 1972, Rordorf 1987)

Boiling Point (°C):

487.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

215.5 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

92.1 (Rordorf 1987)

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

143.238 (Rordorf 1987)

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

48.1 (Rordorf 1987)

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

94 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C, F:

Water Solubility (g/m³ or mg/L at 25°C):

0.00187 (calculated-SOFA model, Govers & Krop 1998)

1.71 × 10⁻³, 1.87 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

6.80 × 10⁻⁹, 5.9 × 10⁻⁷, 2.7 × 10⁻⁵, 7.5 × 10⁻⁴, 1.40 × 10⁻² (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.41 × 10⁻⁶ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)

1.35 × 10⁻⁶, 1.41 × 10⁻⁶ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

0.479; 0.0282 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

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

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

7.84; 7.73 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.85; 7.05, 7.26, 6.96, 7.30 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

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

Bioconcentration Factor, log BCF:

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

Sorption Partition Coefficient, log K_{OC} :

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

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

Volatilization:

Photolysis: photolytic $t_{1/2} = 47$ h when exposed to sunlight in hexane solution (Doobs & Grant 1979); solution photolysis $t_{1/2} = 764$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 7870$ min on a clean glass surface under the same conditions (Nestrick et al. 1980)

Hydrolysis:

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

$k_{OH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (4.6 - 10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.5\text{--}3.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

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

$k_1 = 88, 82 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.62, > 0.8 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}$, $299 \text{ L kg}^{-1} \text{ d}^{-1}$ (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: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991)

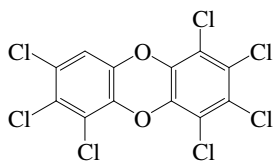
Surface water:

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}100$ yr in sediment for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100$ yr in soil or all homologues (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 1.1$ d for PBO treated and $t_{1/2} < 0.9$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.24 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4,6,7,8-H₇CDD

Chemical Name: 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin

CAS Registry No: 35822-46-9

Molecular Formula: Cl₇C₆H₂O₂Cl₄

Molecular Weight: 425.308

Melting Point (°C):

264–265 (Rordorf 1987,1989; Delle Site 1997)

Boiling Point (°C):

507.2 (Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

218.32 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

92.5 (Rordorf 1987)

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

149.792 (Rordorf 1987)

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

53.9 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

30.42 (Friesen & Webster 1990)

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

100 (Rordorf 1987,1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F: 0.00442 (assuming ΔS_{fus} = 56 J/mol K and mp at 265°C)

0.00423 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)

6.11 × 10⁻⁵ (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.40 × 10⁻⁶*, 2.42 × 10⁻⁶ (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, calculated, Friesen et al. 1985)

2.30 × 10⁻⁶* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)

log [S_L/(mol/L)] = 0.391 – 2820/(T/K) (supercooled liquid, Passivirta et al. 1999)

3.15 × 10⁻⁴ (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

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

7.5 × 10⁻¹⁰* (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987,1989)

3.20 × 10⁻⁸ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

1.02 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)

1.19 × 10⁻⁶ (supercooled liquid, GC/MS, Eitzer & Hites 1989)

3.20 × 10⁻⁹ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

4.41 × 10⁻⁹, 5.15 × 10⁻⁹ (solid P_s, calculated from reported P_L, Delle Site 1997)

8.97 × 10⁻⁶ (corrected supercooled liquid P_L, Eitzer & Hites 1998)

6.03 × 10⁻⁷; 5.89 × 10⁻⁷ (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

8.97 × 10⁻⁶; 6.79 × 10⁻¹⁰ (supercooled liquid P_L; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 13.18 - 6661/(T/\text{K})$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 7.95 - 3844/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P/\text{Pa}) = 17.10357 - 7820.06/(T/\text{K})$ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 2.04×10^{-7} , 5.89×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

0.133 (calculated-P/C, Shiu et al. 1988)
 4.25 (computed-expert system SPARC, Kollig 1995)
 0.832 (calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 7.56 - 7024/(T/\text{K})$ (Passivirta et al. 1999)
 0.275; 0.832 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

11.29, 11.42, 11.90; 11.03, 11.50, 11.98 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 11.05, 11.50 (HPLC-RT correlation, Sarna et al. 1984)
 11.38, 10.55; 11.05, 9.69 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 8.20 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 11.03 (Hansch et al. 1995)
 8.85 (computed-expert system SPARC, Kollig 1995)
 8.40 (calculated-SOFA model, Govers & Krop 1998)
 8.31 (estimated-solubility S_L and regression eq. using lit. K_{ow} values, Passivirta et al. 1999)
 8.051 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 8.27; 8.40 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
 7.66, 7.43, 8.18, 7.73 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

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

Additional data at other temperatures designated * are compiled at the end of this section:

11.42*; 10.73 (generator column-GC, measured range 20–50°C, calculated, Harner et al. 2000)
 $\log K_{OA} = -3.51 + 4450/(T/\text{K})$; temp range 30–50°C (Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

3.32, 3.74 (fathead minnow, rainbow trout, steady-state, wet weight, Muir et al. 1985)
 3.32, 4.32 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 2.92, 4.28 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
 4.68 (guppy, Loonen et al. 1994)
 4.68; 4.08 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.68; 4.68; 4.76 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.68; 4.79 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 6.11, 6.34 (fish muscle $\log BCF_L$ calculated from water, calculated from sediment, Wu et al. 2001)

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

6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 5.47 (DOC, De Voogt et al. 1990)
 7.80 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 10.95; 10.0 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

Photolysis:

photolytic $t_{1/2} = 11$ h in *n*-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)
 solution photolysis $t_{1/2} = 1800$ min at 1.0 m from a GE Model sunlamp and surface photolysis $t_{1/2} = 3140$ min on clean soft glass surface under the same conditions (Nestrick et al. 1980)

$t_{1/2} = 30$ h in *n*-hexadecane solution (Mamantov 1984);

first order $k = 1.02 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 56.46$ d in spring; $t_{1/2} = 47.33$ d in summer; $t_{1/2} = 87.86$ d in autumn, $t_{1/2} = 155.79$ d in winter and averaged $t_{1/2}$ 2993 d over full year (Choudhary & Webster 1985b, 1986)

photolysis $k = 1.02 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 191$ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 1.24 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 57$ d in spring, $k = 1.48 \times 10^2 \text{ d}^{-1}$ $t_{1/2} = 47$ d in summer, $k = 0.80 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 88$ d in autumn, $k = 0.45 \times 10^2 \text{ d}^{-1}$ $t_{1/2} = 156$ d in winter (Choudhary & Webster 1989)

sunlight photolysis $k = 0.28 \text{ d}^{-1}$ in filtered and sterilized natural water and $k = 0.019 \text{ d}^{-1}$ in (2:32, v/v) distilled water-acetonitrile solution at 50°N (Friesen et al. 1990)

photolytic $t_{1/2} = 53.4$ for native congener and $t_{1/2} = 32.6$ h in ^{13}C -labeled congener in extract from fly ash (Tysklind & Rappe 1991)

tropospheric lifetime was calculated based on the gas-phase reaction rate constant $k = (4.6\text{--}10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with the OH radicals to be 1.5–2.4 d (Atkinson 1991)

photodegradation rate constant $k = 0.18 \text{ h}^{-1}$ with $t_{1/2} = 3.9$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000)

$t_{1/2} = 83.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{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 PCDD by ozone) is $5.46 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 3.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 4.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a heptachlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 56 \text{ d}^{-1}$; $k_2 = 0.042 \text{ d}^{-1}$ (rainbow trout exposed to concn of 11, 55 pg/L, Muir et al. 1985)

$k_1 = 19 \text{ d}^{-1}$; $k_2 = 0.040 \text{ d}^{-1}$ (fathead minnow exposed to concn of 8, 39 pg/L, Muir et al. 1985)

$k_2 = 0.048 \text{ d}^{-1}$ (fathead minnow, Muir & Yarechewski 1988)

$k_2 = 0.0092 \text{ d}^{-1}$ (fathead minnow, quoted, Opperhuizen & Sijm 1990)

$k_2 = 0.0110 \text{ d}^{-1}$ (rainbow trout, quoted, Opperhuizen & Sijm 1990)

$k_1 = 32, 150 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.49, > 0.12 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 23 \text{ L kg}^{-1} \text{ d}^{-1}$, $167 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 456 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.081 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0061 \text{ d}^{-1}$ with $t_{1/2} = 49$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime $\tau = 4.4$ d for a hepta-PCDD for the gas-phase reaction with OH radicals (Atkinson 1991);

suggested $t_{1/2} = 1500$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000);

first-order photodegradation $k = 0.19 \text{ h}^{-1}$ with $t_{1/2} = 3.9$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: $t_{1/2} = 11$ h in *n*-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982);

direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 56.46$ d in spring; $t_{1/2} = 47.33$ d in summer; $t_{1/2} = 87.86$ d in autumn; $t_{1/2} = 155.79$ d in winter and averaged $t_{1/2} = 2393$ d over full year (Choudhary & Webster 1985b, 1986);

photolysis $t_{1/2} = 190.97$ h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude: $t_{1/2} = 57$ d in spring, $t_{1/2} = 47$ d in summer, $t_{1/2} = 88$ d in fall and $t_{1/2} = 156$ d in winter (Choudhary & Webster 1989);

$t_{1/2} = 81$ d in sunlit filtered and sterilized surface water and $t_{1/2} = 2.5$ d in surface water of actual pond at 50°N latitude (Friesen et al. 1990);

$t_{1/2} = 53.4$ and 32.6 h in native and ^{13}C -labeled congeners, respectively, in extract from fly ash (Tysklind & Rappe 1991);

suggested $t_{1/2} = 30000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20$ –200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 10$ –100 yr in soil (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} = 17.2$ d in fathead minnow (Adams et al. 1986);

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

$t_{1/2} = 39$ d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);

$t_{1/2} = 27.2$ d in lactating cows (Olling et al. 1991);

half-lives in gold fish: $t_{1/2} = 1.4$ d for PBO treated and $t_{1/2} = 5.6$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.24.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K_{OA}
20	2.40×10^{-6}	7	9.35×10^{-7}	25	7.5×10^{-10}	20	11.66
40	6.30×10^{-5}	11	1.14×10^{-6}	50	8.0×10^{-8}	40	10.774
		17	1.29×10^{-6}	75	4.4×10^{-6}	50	10.225
		21	2.30×10^{-6}	100	1.4×10^{-4}	25	11.42
		26	2.56×10^{-6}	125	2.9×10^{-3}		
		41	6.34×10^{-5}				
		$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 42.4$		$\Delta H_v/(\text{kJ mol}^{-1}) = 92.5$		$\log K_{OA} = a + b/(T/K)$	
		7–41 °C		$\Delta H_{subl}/(\text{kJ mol}^{-1}) = 149.79$		a	–3.51
				$\Delta H_{fus}/(\text{kJ mol}^{-1}) = 53.9$		b	4450
				$\Delta S_{fus}/(\text{J mol}^{-1} \text{K}^{-1}) = 100$		enthalpy of phase change	
						$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 85.10$	

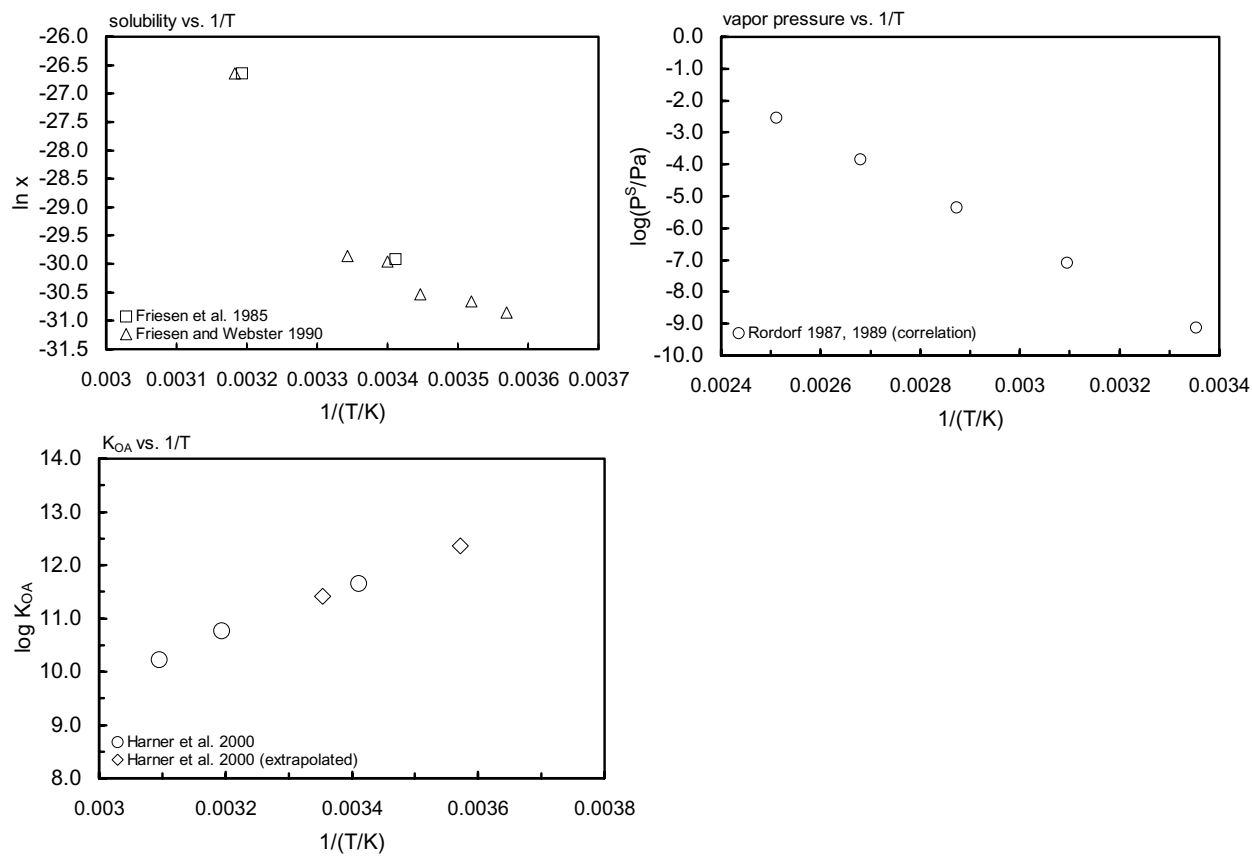
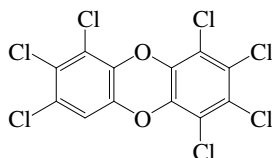


FIGURE 8.1.1.24.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin.

8.1.1.25 1,2,3,4,7,8,9-Heptachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4,7,8,9-H₇CDD

Chemical Name: 1,2,3,4,7,8,9-heptachlorodibenzo-*p*-dioxin

CAS Registry No:

Molecular Formula: Cl₇C₆H₂O₂Cl₄

Molecular Weight: 425.308

Melting Point (°C):

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

222.55 (calculated-liquid density, Govers et al. 1990)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

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

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

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

Fugacity Ratio at 25°C, F:

Water Solubility (g/m³ or mg/L at 25°C):

4.57 × 10⁻⁴ (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)

3.97 × 10⁻⁴, 4.57 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C):

3.39 × 10⁻⁷ (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)

2.57 × 10⁻⁷, 3.39 × 10⁻⁷ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol):

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

0.295; 0.309 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

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

8.22; 8.25 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

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

Bioconcentration Factor, log BCF:

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

Sorption Partition Coefficient, log K_{OC}:

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

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

Volatilization:

Photolysis: photolytic t_{1/2} = 27 h when exposed to sunlight in hexane solution (Dobbs & Grant 1979)

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

k (oxidative degradation rate constant of water dissolved PCDD by ozone) is $5.46 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 3.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 4.4 \text{ d}$ based on gas phase OH reactions and a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a heptachlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 12 \text{ L kg}^{-1} \text{ d}^{-1}$, $183 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 1.3 \text{ d}^{-1}$, $>3.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 22 \text{ L kg}^{-1} \text{ d}^{-1}$, $167 \text{ L kg}^{-1} \text{ d}^{-1}$ (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: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a hepta-PCDD was calculated to be 4.4 d for the gas-phase reaction with OH radical (Atkinson 1991)

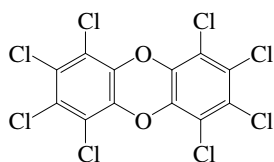
Surface water:

Groundwater:

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

Soil: degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ in soil (estimated, Suzuki et al. 2000)

Biota: half-lives in gold fish: $t_{1/2} = 0.5 \text{ d}$ for PBO treated and $t_{1/2} < 0.2 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.26 Octachlorodibenzo-*p*-dioxin

Common Name: Octachlorodibenzo-*p*-dioxin

Synonym: O₈CDD, OCDD

Chemical Name: octachlorodibenzo-*p*-dioxin

CAS Registry No: 3268-87-9

Molecular Formula: C₁₂Cl₈O₂, Cl₄C₆O₂C₆Cl₄

Molecular Weight: 459.751

Melting Point (°C):

331 (Lide 2003)

Boiling Point (°C):

510 (Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

229.6, 229.11 (calculated-liquid density, crystalline volume, Govers et al. 1990)

237.21 (liquid molar volume, Govers et al. 1995)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.7 (Rordorf 1987)

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

151.13 (Rordorf 1987)

145.7 (Li et al. 2004)

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

61.4 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

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

102 (Rordorf 1986, 1987, 1989; Passivirta et al. 1999)

Fugacity Ratio at 25°C, F: 0.000995 (assuming ΔS_{fus} = 56 J/mol K and mp at 331°C)

0.00107 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1987)

0.00115 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)

3.46 × 10⁻⁶ (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.0 × 10⁻⁶ (Barrie et al. 1983)

4.0 × 10⁻⁷ (¹⁴C-labeled, generator column-HPLC/LSC, Webster et al. 1983)

4.0 × 10^{-7*} (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)

4.0 × 10^{-7*} (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Webster et al. 1985)

1.8 × 10⁻⁴ (Opperhuizen 1986)

1.0 × 10⁻⁷ (¹⁴C-labeled-LSC, Srinivasan & Fogler 1987)

7.4 × 10^{-8*} (extrapolated, generator column-GC/ECD, measured range 40–80°C, Doucette & Andren 1988a)

S/(mol/L) = 8.32 × 10⁻⁶ exp(0.041·t/°C) (generator column-GC/ECD, temp range 40–80°C, Doucette & Andren 1988a)

log x = -3891/(T/K) - 1.482; temp range 40–80°C (generator column-GC/ECD, Doucette & Andren 1988a)

log [S_L/(mol/L)] = -0.163 - 3212/(T/K) (supercooled liquid, Passivirta et al. 1999)

1.03 × 10⁻⁴ (supercooled liquid S_L, GC-RI correlation; Wang & Wong 2002)

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

- 2.40×10^{-5} , 1.8×10^{-5} (quoted, calculated-volatilization rate, Dobbs & Cull 1982)
- 8.70×10^{-6} (20°C, gas saturation, Webster et al. 1985)
- 1.10×10^{-10} * (gas saturation, Rordorf 1985a,b, 1986a,b, 1987, 1989)
- 2.51×10^{-10} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf 1986)
- 2.74×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988)
- 2.77×10^{-7} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1991)
- 2.72×10^{-7} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)
- 0.000280* (120.1°C, average value, gas saturation-GC, measured range 120.1–199.7°C, Rordorf 1990)
- 1.60×10^{-10} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substituted no. plot, Rordorf et al. 1990)
- 2.62×10^{-10} , 2.56×10^{-10} (solid P_s , calculated from reported P_L , Delle Site 1997)
- 2.75×10^{-7} (correcting supercooled liquid P_L value of 1988, Eitzer & Hites. 1998)
- 1.82×10^{-7} ; 1.35×10^{-7} (supercooled liquid P_L , quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 2.75×10^{-7} ; 4.92×10^{-12} (supercooled liquid P_L ; converted to solid P_s with fugacity ratio F , Passivirta et al. 1999)
- $\log(P/\text{Pa}) = 15.81886 - 7629.38/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.0912* (175°C, Knudsen effusion method, measured range, 175–220°C, Li et al. 2002)
- $\log(P_s/\text{Pa}) = 13.62 - 7429/(T/K)$ (solid, Passivirta et al. 1999)
- $\log(P_L/\text{Pa}) = 8.32 - 4221/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
- $\ln(P/\text{Pa}) = (32.825 \pm 0.153) - (15773 \pm 72)/(T/K)$; temp range 448–493 K (Knudsen effusion method, Li et al. 2002)
- 6.61×10^{-8} (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)
- $\ln(P/\text{Pa}) = 38.156 - 16431/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
- $\ln(P/\text{Pa}) = (36.461 \pm 1.020) - (17529 \pm 487)/(T/K)$; temp range 463–493 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

- 0.683 (calculated-P/C, Shiu et al. 1987,1988)
- 1.32; 0.513 (supercooled liquid P_L , quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- $\log[H/(\text{Pa m}^3/\text{mol})] = 8.34 - 1009/(T/K)$ (Passivirta et al. 1999)
- 0.191; 0.513 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

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

- 8.50 (Bruggeman et al. 1984; quoted, Opperhuizen 1986)
- 12.21, 12.60, 12.97; 11.82, 12.72, 13.08 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 11.16, 12.72 (HPLC-RT correlation, Sarna et al. 1984)
- 10.56, 7.53 (calculated-TSA, Doucette 1985)
- 12.26, 11.35; 11.76, 10.07 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 8.60 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 7.59 (generator column-GC/ECD, Doucette & Andren 1987)
- 7.83 (HPLC-RT correlation, Doucette and Andren 1988b)
- 8.60 (calculated, Endicott & Cook 1994)
- 7.59, 8.60 (quoted, Hansch et al. 1995)
- 9.31 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 8.450 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 8.48 (GC-RI correlation, Wang & Wong 2002)

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

- 10.80 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
- 13.0 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

- 1.93, 3.35 (fathead minnow; rainbow trout, steady-state, wet weight, Muir et al. 1985,1986)
- 1.53–2.13; 3.35 (fathead minnow, rainbow trout, Muir et al. 1986)

- 1.00, 2.05 (human fat, calculated-lipid base, Geyer et al. 1987)
 0.903, 1.93 (human fat, calculated-wet wt. base, Geyer et al. 1987)
 1.90, 3.10 (guppy: in whole fish, in lipid, Gobas et al. 1987)
 6.33; 5.85 (plant parts, calculated-vapor pressure; calculated-vapor pressure & HLC, Reischl et al. 1989)
 2.85, 3.97 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990; quoted, Devillers et al. 1996)
 2.85 (predicted for biota held in lake enclosures exposed to water concentration of 0.1 ng/g for 0–10 d, Servos et al. 1992b)
 2.15 (caged invertebrates exposed to water concn. 2.0 ng/L for 0–10 d, Servos et al. 1992b)
 2.32 (caged unionid clams exposed to water concn. 2.9 ng/L for 0–10 d, Servos et al. 1992b)
 2.32 (caged white suckers gill exposed to water concn. 2.9 ng/L for 0–10 d, Servos et al. 1992b)
 1.89 (caged white suckers carcass exposed to water concn. 1.1 ng/L for 0–10 d, Servos et al. 1992b)
 2.42 (caged invertebrates exposed to water concn. 0.6 ng/L for 14–24 d, Servos et al. 1992b)
 2.34 (caged unionid clams exposed to water concn. 0.5 ng/L for 14–24 d, Servos et al. 1992b)
 2.75 (caged white suckers gill exposed to water concn. 1.3 ng/L for 14–24 d, Servos et al. 1992b)
 2.24 (caged white suckers carcass exposed to water concn. 0.4 ng/L for 14–24 d, Servos et al. 1992b)
 3.97 (caged white suckers gill exposed to water concn. 2.8 ng/L for 0–104 d, Servos et al. 1992b)
 3.95 (caged white suckers carcass exposed to water concn. 2.7 ng/L for 0–104 d, Servos et al. 1992b)
 4.13; 3.38 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.13; 4.34; 4.38 (guppy, 21-d exposure, lipid wt basis: measured- $C_{\text{fish}}/C_{\text{W}}$; calculated; rate constant ratio k_1/k_2 from nonlinear regression analysis, Loonen et al. 1994b)
 3.38 (*Poecilia reticulata*, quoted, Devillers et al. 1996)
 4.13; 4.39 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 7.15, 8.45 (fish 5% lipid: BCF_{W} , BCF_{L} , Geyer et al. 2000)
 8.02, 7.53 (fish muscle log BCF_{L} calculated from water, sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 5.92 (estimated DOC partition coeff., Muir et al. 1985)
 7.08 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 5.92 (DOC, De Voogt et al. 1990)
 7.90 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 10.96; 10.5 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

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

Volatilization:

Photolysis:

- photolytic $t_{1/2} = 16$ h by both natural sunlight and fluorescent black light in hexane solution, (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)
 solution photolysis $t_{1/2} = 1460$ min at 1.0 m from a GE Model RS sunlamp and surface photolysis of 46900 min on clean soft glass surface under the same conditions (Nestrick et al. 1980);
 photolysis $t_{1/2} = 24.3$ h in hexadecane solution (Mamantov 1984)
 photolysis $k = 1.06 \times 10^{-6} \text{ s}^{-1}$ in water acetonitrile (2:3, v/v) solution at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 20.53$ d in spring; $t_{1/2} = 17.85$ d in summer; $t_{1/2} = 31.26$ d in autumn; $t_{1/2} = 50.45$ d in winter; and $t_{1/2} = 863$ d averaged over full year (Choudhary & Webster 1986; quoted, Muto et al. 1991)
 photolysis rate constant $k = 1.06 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 183.95$ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 3.45 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 21$ d in spring, $k = 3.97 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 18$ d in summer, $k = 2.27 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 31$ d in fall, $k = 1.40 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 50$ d in winter (Choudhary & Webster 1989)
 photolysis decay rate constants when irradiated with UV light at 254 nm: $k(\text{calc}) = 1.77 \times 10^{-5} \text{ s}^{-1}$, $4.62 \times 10^{-5} \text{ s}^{-1}$ for fly ash suspensions in distilled water, $k(\text{calc}) = 1.42 \times 10^{-5} \text{ s}^{-1}$ for fly ash suspensions in water-acetonitrile solution (2:3, v/v), and $k(\text{calc}) = 2.74 \times 10^{-5} \text{ s}^{-1}$ for fly ash suspensions in water-acetonitrile solution (2:3, v/v) with ozone (Muto et al. 1991);

photolytic $t_{1/2} = 37.3$ h-native congener, $t_{1/2} = 29.6$ h for ^{13}C -labeled congener in extract of fly ash and in tetradecane solution (Tysklind & Rappe 1991);

photolysis $k = 1.6 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 440$ min in pure water, and $k = 1.0 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 680$ min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000);

photodegradation $k = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 5.8$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000)

$t_{1/2} = 105$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{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 OCDD by ozone) is $1.51 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 1.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 9.6$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for OCDD at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 142 \text{ d}^{-1}$; $k_2 = 0.053 \text{ d}^{-1}$ (fathead minnow, flow-through system, Muir et al. 1985; quoted, Adams et al. 1986)

$k_1 = 11 \text{ d}^{-1}$; $k_2 = 0.12 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_1 = 17, 5.0 \text{ d}^{-1}$; $k_2 = 0.103, 0.142 \text{ d}^{-1}$ (rainbow trout exposed to concn of 20, 415 ng/L, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)

$k_1 = 142 \text{ d}^{-1}$; $k_2 = 0.053 \text{ d}^{-1}$ (fathead minnow exposed to concn of 9 ng/L, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)

$k_2 = 0.046 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

$k_1 = 984 \text{ d}^{-1}$; $k_2 = 1.4 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

$k_1 = 60 \text{ d}^{-1}$; $k_2 = 0.12 \text{ d}^{-1}$ (filter-feeder, Servos et al. 1992b)

$k_1 = 30 \text{ d}^{-1}$; $k_2 = 0.08 \text{ d}^{-1}$ (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

$k_1 = 275 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 119 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994)

$k_2 = 0.0053 \text{ d}^{-1}$ with $t_{1/2} = 57$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: atmospheric lifetime of ~7–8 h for reaction with hydroxyl radicals (Atkinson 1987);

estimated reaction $k = 0.0015 \text{ h}^{-1}$ (Paterson et al. 1990);

photodegradation $t_{1/2} = 270$ h in a rotary photo-reactor adsorbed to clean silica gels by filtered $\lambda < 290$ nm of light (Koester & Hites 1992);

tropospheric lifetime $\tau = 9.6$ d, calculated based on gas-phase reaction with OH radicals (Atkinson 1991);

suggested $t_{1/2} = 3950$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000);

first-order photodegradation $k = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 5.8$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: first order photolytic rate constant $k < (0.3 - 2.7) \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 7 - 16$ h exposed to sunlight in hexane solution (Dobbs & Grant 1979);

direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 20.53$ in spring, $t_{1/2} = 17.85$ d in summer; $t_{1/2} = 31.26$ d in fall; $t_{1/2} = 50.45$ d in winter and $t_{1/2} = 853.22$ d averaged over full year (Choudhary & Webster 1986);

$k = 1.064 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhary & Webster 1985a, 1986);

photolysis $t_{1/2} = 183.95$ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct photolysis half-lives near water bodies at 40°N latitude: $t_{1/2} = 21$ d in spring, $t_{1/2} = 18$ d in summer, $t_{1/2} = 31$ d in fall and $t_{1/2} = 50$ d in winter (Choudhary & Webster 1989);

$t_{1/2} = 4.0$ d in the water column of an experimental lake in northwestern Ontario (Servos et al. 1989);

transformation $k(\text{calc}) = 1.6 \times 10^{-3} \text{ h}^{-1}$ in simulated lake enclosure (Servos et al. 1992a);

photolysis $k = 1.6 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 440$ min in pure water, and $k = 1.0 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 680$ min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000);

suggested $t_{1/2} = 79000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: estimated reaction $k = (5.0 \times 10^{-3} - 1.0 \times 10^{-6}) \text{ h}^{-1}$ (Paterson et al. 1990);

$t_{1/2}(\text{calc}) = 10$ yr with a transformation rate constant $k = 7.9 \times 10^{-6} \text{ h}^{-1}$ (Servos et al. 1992a)

$t_{1/2} = 0.2 - 142$ yr (Geyer et al. 2000)

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

suggested $t_{1/2} = 130000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: undergoes photoreduction on soil surfaces to lower chlorinated congeners (Kieatiwong et al. 1990);

estimated reaction $k = 7.0 \times 10^{-7} \text{ h}^{-1}$ (Paterson et al. 1990)

$t_{1/2} > 10$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 10-100$ yr in soil (estimated, Suzuki et al. 2000)

suggested $t_{1/2} = 130000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2} \sim 21$ d from rat (Norback et al. 1975; quoted, Birnbaum 1985);

elimination $t_{1/2} = 13.9$ d for fathead minnow (Muir et al. 1985, Adams et al. 1986);

elimination $t_{1/2} = 5-13$ d for both rainbow trout and fathead minnow (Muir et al. 1986);

mean biological $t_{1/2} \sim 15$ d in rainbow trout (Niimi 1986);

$t_{1/2} = 15$ d in rainbow trout (Niimi & Oliver 1986; quoted, Muir et al. 1986,1990);

$t_{1/2} = 57$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.26.1

Reported aqueous solubilities of octachlorodibenzo-*p*-dioxin at various temperatures

Webster et al. 1985		Friesen et al. 1985		Doucette & Andren 1988a	
generator column-HPLC/LSC		generator column-HPLC/LSC		generator column-GC/ECD	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	4.0×10^{-7}	20	4.0×10^{-7}	40	3.11×10^{-7}
40	2.0×10^{-6}	40	2.0×10^{-6}	60	1.82×10^{-6}
				80	7.87×10^{-6}

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 74.5$
at $40-80^{\circ}\text{C}$

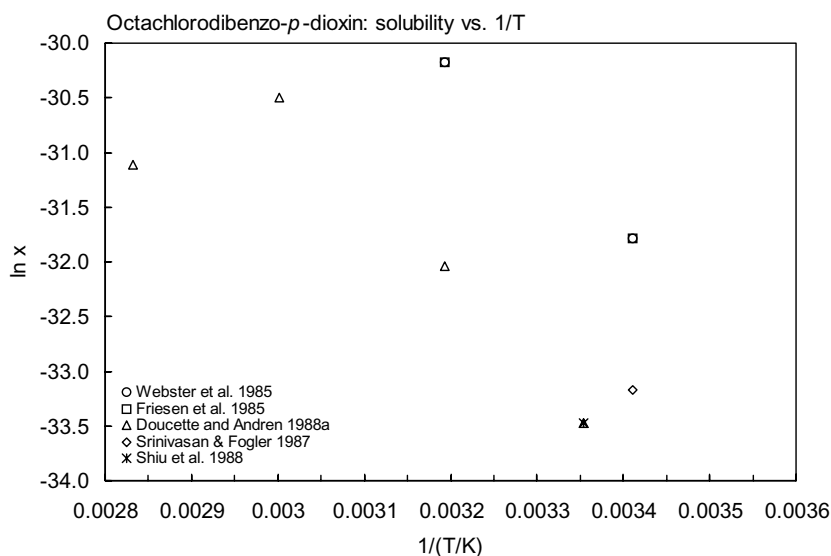


FIGURE 8.1.1.26.1 Logarithm of mole fraction solubility versus reciprocal temperature for octachlorodibenzo-*p*-dioxin.

TABLE 8.1.1.26.2

Reported vapor pressures of octachlorodibenzo-*p*-dioxin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(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)			
Rordorf 1987, 1989		Rordorf 1990		Li et al. 2002	
gas saturation-GC		gas saturation-GC		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
average					
25	1.1×10^{-10}	120.1	0.000280	175	0.0912
50	1.3×10^{-8}	124.9	0.000447	180	0.141
75	7.2×10^{-7}	129.9	0.000737	185	0.204
100	2.4×10^{-5}	134.9	0.00125	190	0.291
125	5.1×10^{-4}	139.9	0.00209	195	0.416
		144.8	0.00352	200	0.607
$\Delta H_v/(\text{kJ mol}^{-1}) = 86.7$		149.8	0.00581	205	0.838
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 151.13$		154.7	0.00949	210	1.20
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 61.4$		159.7	0.0153	215	1.67
$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 102$		165.0	0.0253	220	2.32
		170.0	0.0406		
		175.0	0.0654	eq. 1	P/Pa
		180.0	0.1023	A	32.825
		185.0	0.1585	B	15773
		189.8	0.2515		
		194.7	0.383		
		199.7	0.584		
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 149.822$			
		120 – 200 °C			

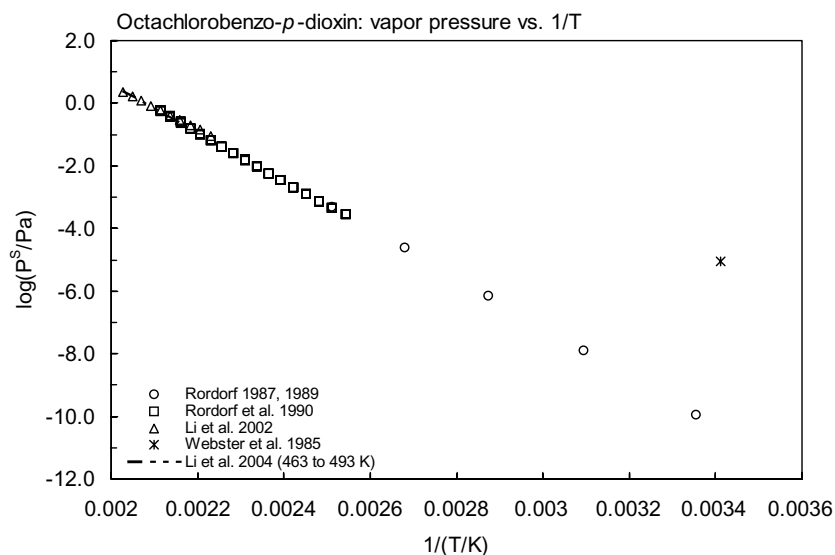


FIGURE 8.1.1.26.2 Logarithm of vapor pressure versus reciprocal temperature for octachlorodibenzo-*p*-dioxin.

8.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 8.2.1

Summary of physical properties of some chlorinated dioxins

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol	
							from ρ ^(a)	Le Bas
Dibenzo- <i>p</i> -dioxin	262-12-4	C ₁₂ H ₈ O ₂	184.191	120.5		0.116	143.82	177.0
1-Chloro-	39227-53-7	C ₁₂ H ₇ O ₂ Cl	218.636	105.5		0.162	157.41	197.9
2-Chloro-	39227-54-8	C ₁₂ H ₇ O ₂ Cl	218.636	89		0.236	154.85	197.9
2,3-Dichloro-	29446-15-9	C ₁₂ H ₆ O ₂ Cl ₂	253.081	164	358	0.0433	164.07	218.8
2,7-Dichloro-	33857-26-0	C ₁₂ H ₆ O ₂ Cl ₂	253.081	201	374.5	0.0188	165.88	218.8
2,8-Dichloro-	38964-22-6	C ₁₂ H ₆ O ₂ Cl ₂	253.081	151		0.0580	165.88	218.8
1,2,4-Trichloro-	39227-58-2	C ₁₂ H ₅ O ₂ Cl ₃	287.526	129	375	0.0954	179.66	239.7
1,3,7-Trichloro-	67026-17-5	C ₁₂ H ₅ O ₂ Cl ₃	287.526	148.5	398	0.0614	179.11	239.7
2,3,7-Trichloro-	33857-28-2	C ₁₂ H ₅ O ₂ Cl ₃	287.526	162–163	408.4	0.0448	175.10	239.7
1,2,3,4-Tetrachloro-	30746-58-8	C ₁₂ H ₄ O ₂ Cl ₄	321.971	189	419	0.0246	186.71	260.6
1,2,3,7-Tetrachloro-	67028-18-6	C ₁₂ H ₄ O ₂ Cl ₄	321.971	172	438.3	0.0361	186.52	260.6
1,2,7,8-Tetrachloro-	34816–53–0	C ₁₂ H ₄ O ₂ Cl ₄	321.971				186.88	260.6
1,3,6,8-Tetrachloro-	30746-58-8	C ₁₂ H ₄ O ₂ Cl ₄	321.971	219	438.3	0.0125	192.34	260.6
1,3,7,8-Tetrachloro-	50585-46-1	C ₁₂ H ₄ O ₂ Cl ₄	321.971	193.5–195	438.3	0.0218	188.33	260.6
1,3,7,9-Tetrachloro-	62470-53-5	C ₁₂ H ₄ O ₂ Cl ₄	321.971				192.34	260.6
2,3,7,8-Tetrachloro-	1746-01-6	C ₁₂ H ₄ O ₂ Cl ₄	321.971	295		0.00224	184.32	260.6
1,2,3,4,7-Pentachloro-	39227-61-7	C ₁₂ H ₃ O ₂ Cl ₅	356.416	195	464.7	0.0215	197.74	281.5
1,2,3,7,8-Pentachloro-	40321-76-4	C ₁₂ H ₃ O ₂ Cl ₅	356.416		464.7		195.74	281.5
1,2,4,7,8-Pentachloro-	58802-08-7	C ₁₂ H ₃ O ₂ Cl ₅	356.416	206	464.7	0.0168	199.91	281.5
1,2,3,4,7,8-Hexachloro-	39227-26-8	C ₁₂ H ₂ O ₂ Cl ₆	390.861	273	487.7	0.00369	206.96	302.4
1,2,3,6,7,8-Hexachloro-	57653-85-7	C ₁₂ H ₂ O ₂ Cl ₆	390.861	285	487.7	0.00281	207.16	302.4
1,2,3,7,8,9-Hexachloro-	19408-74-3	C ₁₂ H ₂ O ₂ Cl ₆	390.861	243–244	487.7	0.00718	207.16	302.4
1,2,4,6,7,9-Hexachloro-	39227-62-8	C ₁₂ H ₂ O ₂ Cl ₆	390.861	238–240	487.7	0.00795	215.50	302.4
1,2,3,4,6,7,8-Heptachloro-	35822-46-9	C ₁₂ HO ₂ Cl ₇	425.308	265	507.2	0.00442	218.38	323.3
1,2,3,4,7,8,9-Heptachloro-		C ₁₂ HO ₂ Cl ₇	425.308				222.55	323.3
Octachloro-	3268-87-9	C ₁₂ O ₂ Cl ₈	459.751	331	510	0.000995	229.60	344.2

*Assuming ΔS_{fus} = 56 J/mol K; (a) Govers et al. 1990 (at 25°C).

TABLE 8.2.2

Selected physical-chemical properties of some chlorinated dioxins at 25°C

Compound	Selected properties					log K _{OW}	Henry's law constant
	Vapor pressure		Solubility				H/(Pa·m ³ /mol)
	P ^S /Pa	P _L /Pa	S/(mg/m ³)	C ^S /(mmol/m ³)	C _L /(mmol/m ³)		calculated P/C
Dibenzo- <i>p</i> -dioxin	0.055	0.474	865	4.696	40.48	4.30	11.71
1-CDD	0.012	0.074	417	1.907	11.77	4.75	6.292
2-CDD	0.017	0.0730	295	1.350	5.717	5.00	12.60
2,3-DCDD	0.00039	0.00901	14.9	0.0589	1.360		6.624
2,7-DCDD	0.00012	0.00811	3.75	0.0148	0.788	6.38	8.098
2,8-DCDD	0.00014	0.00241	16.7	0.0660	1.138		2.122
1,2,4-T ₃ CDD	0.0001	0.00105	8.41	0.0293	0.306		3.419
1,2,3,4-T ₄ CDD	6.40 × 10 ⁻⁶	2.60 × 10 ⁻⁴	0.55	0.0017	0.0694	6.60	3.747
1,2,3,7-T ₄ CDD	1.00 × 10 ⁻⁶	2.77 × 10 ⁻⁵	0.42	0.0013	0.0361	6.90	0.766
1,3,6,8-T ₄ CDD	7.00 × 10 ⁻⁷	5.60 × 10 ⁻⁵	0.32	0.000994	0.0795	7.18	0.704
2,3,7,8-T ₄ CDD	2.00 × 10 ⁻⁷	8.93 × 10 ⁻⁵	0.0193	0.00006	0.0268	6.80	3.336
1,2,3,4,7-P ₅ CDD	8.80 × 10 ⁻⁸	4.09 × 10 ⁻⁶	0.118	0.000331	0.0154	7.40	0.266
1,2,3,4,7,8-H ₆ CDD	5.10 × 10 ⁻⁹	1.38 × 10 ⁻⁶	0.006	1.54 × 10 ⁻⁵	0.00416	7.80	0.332
1,2,3,4,6,7,8-H ₇ CDD	7.50 × 10 ⁻¹⁰	1.70 × 10 ⁻⁷	0.0024	5.64 × 10 ⁻⁶	0.00128	8.00	0.133
OCDD	1.10 × 10 ⁻¹⁰	1.11 × 10 ⁻⁷	0.000074	1.61 × 10 ⁻⁷	0.00016	8.20	0.683

TABLE 8.2.3

Suggested half-life classes of polychlorinated dibenzo-*p*-dioxins in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Dibenzo- <i>p</i> -dioxin	3	3	6	7
2-CDD	4	4	7	8
2,7-DCDD	4	4	7	8
2,8-DCDD	4	4	7	8
1,2,4-T ₃ CDD	4	4	7	8
1,2,3,4-T ₄ CDD	4	5	8	9
2,3,7,8-T ₄ CDD	4	5	8	9
1,2,3,4,7-P ₅ CDD	5	5	8	9
1,2,3,4,7,8-H ₆ CDD	5	6	9	9
1,2,3,4,6,7,8-H ₇ CDD	5	6	9	9
OCDD	5	7	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55888 (~ 6 years)	> 30,000

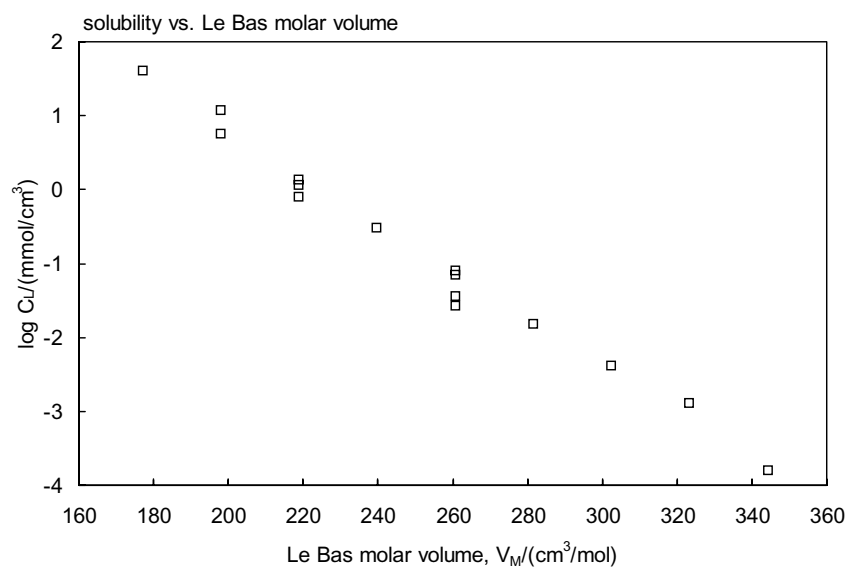


FIGURE 8.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

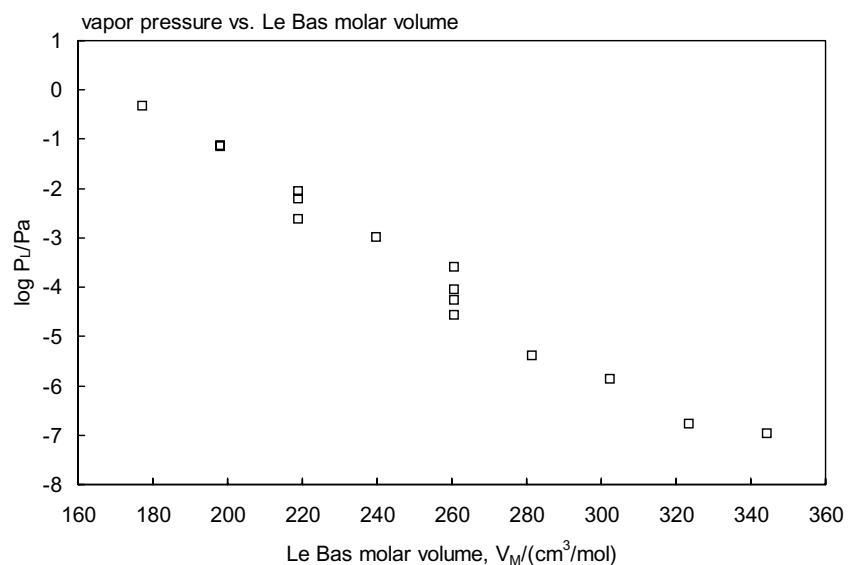


FIGURE 8.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

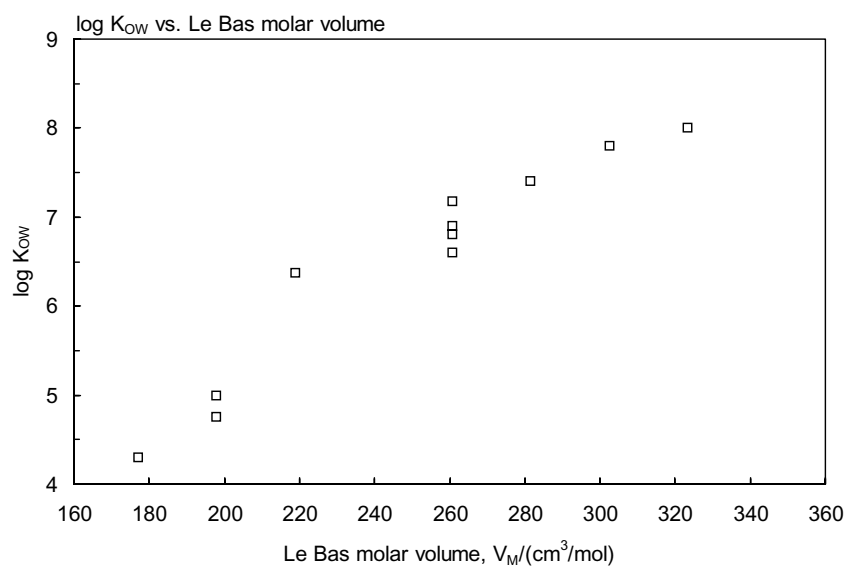


FIGURE 8.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

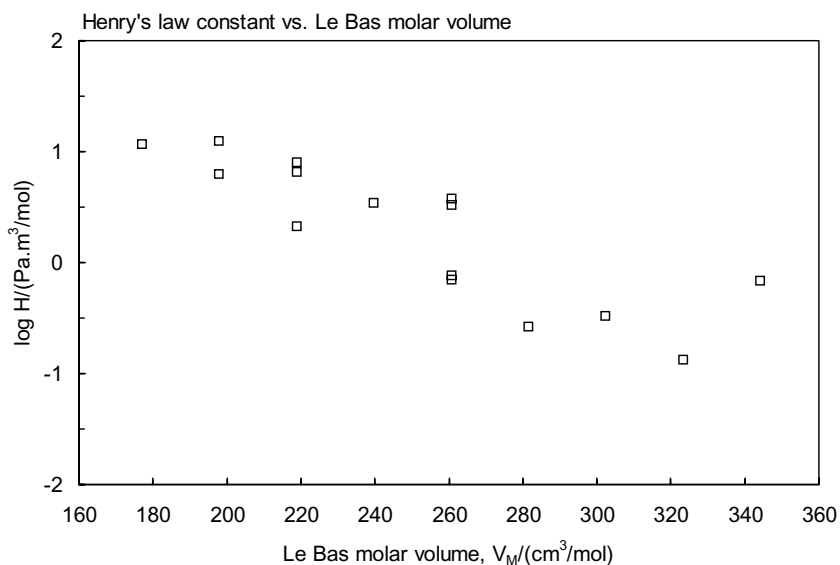


FIGURE 8.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

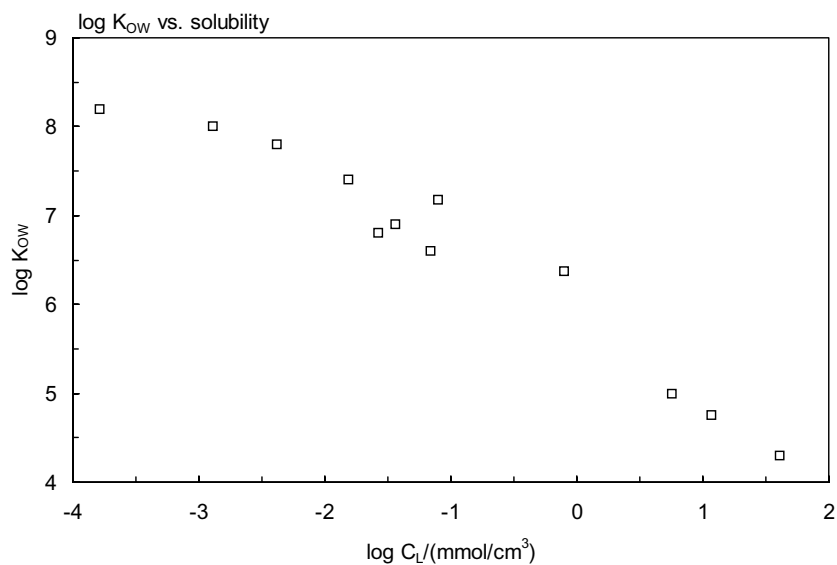


FIGURE 8.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated dibenzo-*p*-dioxins.

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