Excerpts from the
ILLUSTRATED HANDBOOK
OF PHYSICAL-CHEMICAL PROPERTIES
AND ENVIRONMENTAL FATE FOR ORGANIC CHEMICALS

Volume II
Polynuclear Aromatic Hydrocarbons,
Polychlorinated Dioxins,
and Dibenzofurans

NATIONAL LABORATORY
MAY 27 1993

Donald Mackay
Wan Ying Shiu
Kuo Ching Ma

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### 3.1 List of Chemicals and Data Compilations:

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<td>1,2,3,4,7-Pentachloro-dibenzo-p-dioxin</td>
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<td>1,2,3,4,6,7,8-Heptachloro-dibenzo-p-dioxin</td>
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### 3.2 Summary Tables and QSAR Plots

### 3.3 Illustrative Fugacity Calculations: Level I, II and III

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| 2-Chlorodibenzo-p-dioxin       | 436 |
| 2,7-Dichlorodibenzo-p-dioxin   | 440 |
| 2,8-Dichlorodibenzo-p-dioxin   | 444 |
| 1,2,4-Trichlorodibenzo-p-dioxin| 448 |
| 1,2,3,4-Tetrachlorodibenzo-p-dioxin| 452 |
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| 1,2,3,4,7-Pentachlorodibenzo-p-dioxin| 460 |
| 1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin| 464 |
| 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin| 468 |
| Octachloro-dibenzo-p-dioxin    | 472 |

### 3.4 Commentary on the Physical-Chemical Properties and Environmental Fate

### 3.5 References

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3.1 List of Chemicals and Data Compilations
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: Cl₂C₆H₂O₂C₆H₂Cl₂
Molecular Weight: 322.0

Melting Point (°C):
- 320-325 (quoted, Pohland & Yang 1972; Merck Index 1989)
- 303-305 (Crummett & Stehl 1973; quoted, Callahan et al. 1979; Mabey et al. 1982; Mill 1985)
- 306 (Branson et al. 1985; Crosby 1985)
- 305-0 (quoted, Schroy et al. 1985a; Shiu et al. 1988)

Boiling Point (°C):
- 421.2 (Schroy et al. 1985a)

Density (g/cm³ at 20°C):
- 1.827 (solid at 25°C, Schroy et al. 1985a)
- 1.021 (liquid at normal boiling point, Schroy et al. 1985a)

Molar Volume (cm³/mol):
- 275.6 (LeBas method, Shiu et al. 1988)
- 137.10 (calculated as per Pearlman 1986, De Voogt et al. 1990)
- 134.40 (calculated as per Govers & De Voogt 1989, De Voogt et al. 1990)
- 1.508 (intrinsic Vₜ/100, Hawker 1990)
- 184.32, 184.97 (calculated-liquid density, crystalline volume, Govers et al. 1990)

Molecular Volume (Å³):
Total Surface Area, TSA (Å²):

Heat of Fusion, ΔHₘₙ kcal/mol:
- 9.30 (quoted, Schroy et al. 1985a,b)

Entropy of Fusion, ΔSₘₙ, cal/mol K (e.u.):
Fugacity Ratio at 25°C (assuming $\Delta S = 13.5$ e.u.):
0.0017  (Shiu et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C):
0.0002  (GC/ECD, Crummett & Stehl 1973; quoted, Callahan et al. 1979; Mabey et al. 1982; Mackay et al. 1985; Mill 1985; Jackson et al. 1986; Shiu et al. 1988)
0.0002  (quoted, Matsumura & Benezet 1973; Isensee & Jones 1975)
0.0002  (quoted, Neely 1979)
0.0002  (quoted, Kenaga 1980)
0.000317 ($^{14}$C-labeled, gen. col.-HPLC/LSC, Webster et al. 1983, quoted, Schroy et al. 1985a; Shiu et al. 1988)
0.0002  (quoted, Branson et al. 1985; Crosby 1985; Mill 1985)
1.93x10⁻⁵ (shake flask-GC/MS, Marple et al. 1986a; quoted, Travis & Hattemer-Frey 1987, Shiu et al. 1988; Walters & Guiseppi-Elie 1988; Kieatiwong et al. 1990)
7.91x10⁻⁶ ($^{14}$C-labeled, Adams & Blaine 1986, quoted, Schroy et al. 1985a,b; Mehrle et al. 1988; Shiu et al. 1988; Mackay 1991)
0.00032  (quoted, Srinivasan & Fogler 1987)
1.93x10⁻⁶ (selected, Shiu et al. 1988, quoted, Paterson et al. 1990)
(1.25-1.93)x10⁻⁴ (quoted, Walters & Giuseppi-Elie 1988)
4.83x10⁻⁴ (17.3°C, gen. col.-GC/MS, Lodge 1989)
7.90x10⁻⁶ (20-22°C, quoted, Lodge 1989)
7.20x10⁻⁶ (quoted, Puri et al. 1989)
0.000192 (20°C, quoted, De Voogt et al. 1990)
0.000688; 0.0081-0.0194 (calculated-QSAR; quoted, Fiedler & Schramm 1990)

Vapor Pressure (Pa at 25°C):
1.33x10⁻⁴ (calculated from structure, Mabey et al. 1982)
1.00x10⁻⁷ ($^{14}$C-gas saturation method, Jaber & Podoll 1983; quoted, Mill 1985)
9.33x10⁻⁸ (quoted, Crosby 1985)
6.00x10⁻⁹ (quoted, Mackay et al. 1985)
9.60x10⁻⁹ (quoted, Mill 1985)
(3.5-6.3)x10⁻⁶ (gas saturation method, Rordorf 1985a,b, 1986,1987,1989; quoted, Shiu et al. 1988)
4.61x10⁻⁷ (30.1°C, gas saturation, Schroy et al. 1985a,b)
2.02x10⁻⁷ (gas saturation method, Schroy et al. 1985b; quoted, Rordorf 1985a,b; Rordorf et al. 1986a,b, 1987,1989,1990; Shiu et al. 1988)
1.51x10⁻⁷ (Schroy et al. 1985a,b; quoted, Shiu et al. 1988)
4.50x10⁻⁷ (Webster et al. 1985; quoted, Shiu et al. 1988)
9.86x10⁻⁸ ($^{14}$C-gas saturation, Podoll et al. 1986; quoted, Shiu et al. 1988; Kieatiwong et al. 1990)
8.14x10⁻⁸, 6.0x10⁻³ (20°C, quoted: solid, subcooled value, Bidleman & Foreman 1987)
<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.50x10^6</td>
<td>(quoted, Travis &amp; Hattemen-Frey 1987)</td>
</tr>
<tr>
<td>6.20x10^7</td>
<td>(calculated, Rordorf 1987, 1989)</td>
</tr>
<tr>
<td>2.00x10^7</td>
<td>(selected, Shiu et al. 1988; quoted, Paterson et al. 1990)</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0021</td>
<td>(calculated-P/C, Mabey et al. 1982)</td>
</tr>
<tr>
<td>0.152</td>
<td>(calculated-P/C, Crosby 1985)</td>
</tr>
<tr>
<td>0.212</td>
<td>(calculated-P/C, Schroy et al. 1985)</td>
</tr>
<tr>
<td>1.64</td>
<td>(calculated-P/C, Podoll et al. 1986)</td>
</tr>
<tr>
<td>1.63, 3.34, 10.34</td>
<td>(calculated-P/C, Shiu et al. 1988)</td>
</tr>
<tr>
<td>0.196</td>
<td>(calculated-P/C form data of Schroy et al. 1985, 1988)</td>
</tr>
<tr>
<td>7.93</td>
<td>(calculated-P/C, Jury et al. 1990)</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.38</td>
<td>(Crummett &amp; Stehl 1973; quoted, Birnbaum 1985)</td>
</tr>
<tr>
<td>6.79</td>
<td>(quoted, Neely 1979; Veith et al. 1979; Corbet et al. 1983)</td>
</tr>
<tr>
<td>6.15</td>
<td>(quoted, Kenaga 1980; Schroy et al. 1985b; Marple et al. 1986)</td>
</tr>
<tr>
<td>7.16</td>
<td>(calculated-f const, Perkow et al. 1980; quoted, Marple et al. 1986; Shiu et al. 1988)</td>
</tr>
<tr>
<td>6.84</td>
<td>(calculated-f const, Johnson 1982; quoted, Mill 1985; Marple et al. 1986; Shiu et al. 1988)</td>
</tr>
<tr>
<td>6.84</td>
<td>(calculated-f const, Mabey et al. 1982)</td>
</tr>
<tr>
<td>6.15</td>
<td>(quoted, Garten &amp; Trabalka 1983)</td>
</tr>
<tr>
<td>5.50</td>
<td>(calculated, Kaiser 1983; quoted, Shiu et al. 1988)</td>
</tr>
<tr>
<td>8.93</td>
<td>(HPLC-RT, Sarna et al. 1984)</td>
</tr>
<tr>
<td>6.15</td>
<td>(quoted, Branson et al. 1985)</td>
</tr>
<tr>
<td>6.845</td>
<td>(quoted, Crosby 1985)</td>
</tr>
<tr>
<td>6.839</td>
<td>(quoted, Mill 1985)</td>
</tr>
<tr>
<td>7.14</td>
<td>(quoted, Mackay et al. 1985)</td>
</tr>
<tr>
<td>8.48</td>
<td>(quoted, Podoll et al. 1986)</td>
</tr>
<tr>
<td>7.16, 6.15-7.28</td>
<td>(calculated-f const., quoted range, Jackson et al. 1986)</td>
</tr>
<tr>
<td>7.02</td>
<td>(HPLC-RT, Burkhard &amp; Kuehl 1986; quoted, Shiu et al. 1988; Sijm et al. 1989a; De Voogt et al. 1990)</td>
</tr>
<tr>
<td>6.64</td>
<td>(quoted average, Marple et al. 1986a; quoted, Geyer et al. 1987)</td>
</tr>
<tr>
<td>6.64</td>
<td>(stirring-GC/MS, Marple et al. 1986b; quoted, Geyer et al. 1987; Shiu et al. 1988; Walters &amp; Giuseppi-Elie 1988)</td>
</tr>
<tr>
<td>7.16</td>
<td>(quoted, Jackson et al. 1986)</td>
</tr>
<tr>
<td>6.85</td>
<td>(quoted, Travis &amp; Hattemer &amp; Frey 1987)</td>
</tr>
<tr>
<td>6.80</td>
<td>(selected, Shiu et al. 1988; quoted, Gobas et al. 1988; Sijm et al. 1989a; Goba &amp; Schrap 1990; Paterson et al. 1990)</td>
</tr>
<tr>
<td>6.80</td>
<td>(quoted, Hawker 1990)</td>
</tr>
<tr>
<td>Bioconcentration Factor, log BCF:</td>
<td></td>
</tr>
<tr>
<td>---------------------------------</td>
<td></td>
</tr>
<tr>
<td>6.42  (slow stirring-GC/MSD, from fly ash extract, Sijm et al. 1989a)</td>
<td></td>
</tr>
<tr>
<td>7.70, 6.60-7.70 (calculated-QSAR; quoted, Fiedler &amp; Schramm 1990)</td>
<td></td>
</tr>
<tr>
<td>6.15  (quoted, Kieatiwong et al. 1990)</td>
<td></td>
</tr>
<tr>
<td>7.10  (calculated, Brom et al. 1991)</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Bioconcentration Factor, log BCF:</th>
</tr>
</thead>
</table>
| 1.69, 2.34, 2.08 (daphnia, ostracod, brine shrimp, 
^{14}C-labeled-LSC, Matsumura & Benezet 1973) |
| 4.53  (calculated-K_{ow}, Neely et al. 1974) |
| 4.30-4.41; 3.6-3.95 (snail, Gambaia, daphnids; duckweed, algae, catfish; 
Isensee & Jones 1975) |
| 5.38  (calculated-K_{ow}, Chou et al. 1977; quoted, Branson et al. 1985) |
| 4.52  (fish, calculated-K_{ow}, Veith et al. 1979; quoted, Corbet et al. 1983) |
| 3.30  (calculated-K_{ow}, Banerjee et al. 1980; quoted, Branson et al. 1985) |
| 3.73, 4.55 (fish: flowing water test, static ecosystem test, Kenaga & Goriag 1980, Kenaga 1980) |
| 5.84  (microorganism, calculated-K_{ow}, Mabey et al. 1982) |
| 3.97  (rainbow trout, Branson et al. 1983; quoted, Adams et al. 1986) |
| -0.15, 0.54, 3.02 (rodents, cow, fish, Garten & Trabalka 1983) |
| 3.30, 5.38, 4.53 (fish: calculated-K_{ow}, Branson et al. 1985) |
| 3.97, 3.67 (rainbow trout: whole body, muscle, Branson et al. 1985) |
| 1.39-1.037, 1.39-0.568 (rats fat, liver, Geyer et al. 1986) |
| 0.544, -0.155 (beef fat, liver, Geyer et al. 1986) |
| 1.394 (cattle, calculated-steady state, Geyer et al. 1986) |
| 1.38-1.60 (rhesus monkey, Geyer et al. 1986) |
| 4.11  (guppy, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990) |
| 2.18  (human fat, calculated, Geyer et al. 1986) |
| 1.079 (dry fodder to milk fat, Connett & Webster 1987; quoted, Webster & Connett 1990) |
| 1.398 (dry fodder to milk fat, Travis & Hattemer-Frey 1987; quoted, Webster & Connett 1990) |
| 2.23, 2.18  (calculated-K_{ow} for human fat: lipid basis, wet weight basis, Geyer et al. 1987) |
| 1.65-4.46, 4.69 (fish: quoted values, average, Travis & Hattemer-Frey 1987) |
| 4.43, 4.59 (rainbow trout: measured average, estimated BCF at steady-state, for 28-days exposure, Mehrle et al. 1988) |
| 0.833  (dry fodder to milk fat, McKone & Ryan 1988; quoted, Webster & Connett 1990) |
| 0.699 (dry fodder to milk fat, Michaels 1989; quoted, Webster & Connett 1990) |
4.30, 5.0 (goldfish after 8 hours exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)

3.89 (fathead minnows, quoted, De Voogt et al. 1990)

4.59 (rainbow trout, quoted, De Voogt et al. 1990)

5.80, 5.90 (goldfish after 6 days 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)

4.11 (fish, quoted, Hawker 1990)

4.63, 4.40 (pine needle/air BCF values, Reissinger et al. 1990)

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)

Sorption Partition Coefficient, log K<sub>OC</sub>:

5.67 (organic carbon soil, calculated-K<sub>ow</sub>, Kenaga 1980; quoted, Puri et al. 1989)

6.52 (sediment, calculated-K<sub>ow</sub>, Mabey et al. 1982)

6.95, 7.39-7.58 (calculated-K<sub>ow</sub>, 10 soils from Missouri & New Jersey, Jackson et al. 1985)

6.04 (calculated-S, Mill 1985)

6.90 (calculated-K<sub>ow</sub>, Mill 1985)

6.22-6.54 (red clay soil from Missouri, Marple et al. 1986)

5.96-6.09 (Alluvial soil from Missouri, Marple et al. 1986)

6.95 (calculated-K<br />_<sub>ow</sub>, Jackson et al. 1986)

4.83 (hydroxy aluminum-clay, Srinivasan & Fogler 1987)

6.60 (¹⁴C-labeled, soil, batch equilibrium, GC/ECD, Walters & Guiseppi-Elie 1988)

6.7-7.0 (calculated from aqueous solubility, Walters & Guiseppi-Elie 1988)

3.06 (soil, Eduljee 1987)

6.30 (sediment from Lake Ontario, Lodge & Cook 1989)

7.59, 7.25 (solids, organic carbon, 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, 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)

5.7, 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 (uncontaminated Time Beach soil/regression analysis of 2-day & 10-day isotherm, Walters et al. 1989)

6.14 (soil, Jury et al. 1990)

6.8 (calculated, Broman et al. 1991)
Half-Lives in the Environment:

Air: dominant transformation process in the atmosphere (Atkinson et al. 1982); 200 hours for OH radical oxidation (Podoll et al. 1986); room temperature gas-phase OH radical reaction rate constant was calculated to be $9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ sec$^{-1}$ corresponding to an atmospheric lifetime of about 3 days (Atkinson 1987a); 22.3-223 hours, based on estimated photooxidation half-life in air (Atkinson 1987b; quoted, Howard et al. 1991); half-life in vapor phase undergo rapid photolysis with an upper limit of 1 hour (Travis & Hattemer-Frey 1987); atmospheric rate constant in summer sunlight at 40°N latitude of 0.012 minute$^{-1}$ with half-life of 58 minutes (Buser 1988); rate constant for photolysis in air at 150-350°C of $5.9 \times 10^3$ sec$^{-1}$ (Orth et al. 1989); reaction rate constant estimated to be 0.02 hour$^{-1}$ (Paterson et al. 1990).

Surface water: photolysis half-life in methanol solution, 3 hours in sunlight (Plimmer et al. 1973); half-life in a model aquatic environment, 600 days (Ward & Matsumura 1978); photolysis in n-hexadecane at 1.0 m from a GE model RS sunlamp, with half-life of 56.8 minutes (Nestrick et al. 1980); reaction rate constant estimated to be $2.6 \times 10^5$ hour$^{-1}$ (Mackay et al. 1985); calculated sunlight photolysis half-lives over four seasons at 40°N latitude averaged over for 24 hours exposure per day: 130 hours in winter, 28 hours in spring, 20 hours in summer and 52 hours in fall (Mill et al. 1982; quoted, Mill 1985); volatilization half-lives of about 32 days for water in ponds, lakes and about 16 days for rivers; calculated photolysis half-lives in sunlight at 40°N latitude: 118 hours in winter, 27 hours in spring, 21 hours in summer and 51 hours in fall (Podoll et al. 1986); photolysis in near-surface waters is an important degradative pathway with half-life of 40 hours (Travis & Hattemer-Frey 1987); sunlight-induced photolysis half-life in isooctane, 14 minutes (Buser 1988); reaction rate constant estimated to be 0.008 hour$^{-1}$ (Paterson et al. 1990); 10032-14160 hours, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: 20064-28320 hours, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment: half-life in aquatic sediment 12000 to 14400 hours (Ward & Matsumura 1978; quoted, Quensen & Matsumura 1983); reaction rate constant estimated to be $8.0 \times 10^4$ hour$^{-1}$ (Mackay et al. 1985); and $1.5 \times 10^4$ hour$^{-1}$ (Paterson et al. 1990); > 1 year (O'Keefe et al. 1986).

Soil: 10032-14160 hours, based on soil disaway test data for two soils (Kearney et al. 1971; quoted, Howard et al. 1991); about one year (Kearney et al. 1973; quoted, Quensen & Matsumura 1983); degradation half-life of 10-12 years in soil (De Domenico et al. 1980, Kimbrough et al. 1984); about 1 year if applied to surface on soil with 2,4-D (Nash & Beall 1980); reaction rate constant estimated to be $8.0 \times 10^4$ hour$^{-1}$ (Mackay et al. 1985); and $1.1 \times 10^5$ hour$^{-1}$ (Paterson et al. 1990); photodegradation is a rapid process at the soil surface with a half-life of 10 minutes during the day (Facchetti et al. 1986); degradation
reaction rate coefficient in soil was considered to be zero (Travis & Hattemer-Frey 1987); half-life in soil about 10 years if TCDD is on or near the surface and 100 years if TCDD is buried at greater depth (Nauman & Schaum 1987); calculated half-life, 10 years (Eduljee 1987); 10 years or longer (Boddington et al. 1990); photolysis in soil is slow (Kieatiwong et al. 1990); half-life for volatilization to atmosphere below surface soil, 365 days (Jury et al. 1990).

Biota: estimated half-life in rat, 31 days (Rose et al. 1976; quoted, Birnbaum 1985); estimated half-life in hamster, 11 days (Olsen et al. 1980; quoted, Birnbaum 1985); estimated half-life in guinea pig, 30 days (Decad et al. 1981a; quoted, Birnbaum 1985); estimated half-life in mouse, 11-24 days (Gasiewicz et al. 1983; quoted, Birnbaum 1985); total body burden depuration half-life of $^{14}$C-TCDD in whole rainbow trout is 58 days (Branson et al. 1983, 1985; quoted, Adams et al. 1986); half-lives: 17-37 days in mouse, 31 days in rat and 30 days in guinea pig (quoted, Van den Berg et al. 1985); elimination half-life of 14.5 days from fathead minnows (Adams et al. 1986; quoted, Niimi & Oliver 1986); 105 days in whole body of rainbow trout (Kleeman et al. 1986; quoted, Muir et al. 1990); 300-325 days in carp (Kuehl et al. 1986); biological half-life for rainbow trout, 58 days (Niimi & Oliver 1986); estimated half-life in human, 5.8 years (Poiger & Schlatter 1986; quoted, Travis & Hattemer-Frey 1987; Webster & Connett 1991); > 336 days for carps in Lake Superior (Kuehl et al. 1987); estimated half-life in human, 6.7 years (Kissel & Robarge 1988; quoted, Webster & Connett 1991); elimination half-lives of 15-48 days from rainbow trout for exposures of different concentrations (Mehrle et al. 1988); estimated half-life in human, 7.1 years (Pirkle et al. 1989; quoted, Webster & Connett 1991); half-lives of 5 to 8 years for human, 17.4-31 days for rats, 9.6-24.4 days for mice, 22-93.7 days for guinea pigs, 12.0-150 days for hamsters, 1 year for monkeys (Boddington et al. 1990); 40.3 days for lactating cows (Olling et al. 1991); assumed half-life for human, 5 to 10 years (Schecter & Ryan 1991); elimination half-life from lake trout sac fry, 35-37 days (Walker et al. 1991); 4.4 years for a 70 kg non-lactating "reference" human (Webster & Connett 1991).

Environmental Fate Rate Constants or Half-Lives:

Volatilization: probably not an important process (Callahan et al. 1979); half-life of 20-200 days from water column which will be slowed down further by the fact that it is sorbed to the sediment and biota (Mills 1985); half-lives of about 32 days for ponds and about 16 days for rivers (Podoll et al. 1986); half-life for volatilization from soil was 104 days by calculation assuming diffusion of TCDD in soil is vapor-dominated up to volumetric water content of 0.3 m$^3$/m$^3$, and then liquid-dominated to saturation (Eduljee 1987); half-life of 190 days (Thibodeaux & Lipsky 1985; quoted, Eduljee 1987); half-life for volatilization from below surface soil is 365 days (Jury et al. 1990).
Photolysis: stable to sunlight with a half-life of 14 days in distilled water (Crosby et al. 1971; quoted, Dougherty et al. 1991); TCDD in methanol solution has a half-life of about 3 hours in sunlight (Plimmer et al. 1973); half-life for vapor in sunlight, 56 minutes (Peterson 1976; quoted, Mill 1985); thin film of TCDD on glass plates showed transformation at about 6 hours (Crosby & Wong 1977); estimated half-life was 320 hours for the reaction with $3 \times 10^{15}$ mole OH radicals in vapor phase in atmosphere with rate constant of $6 \times 10^{-7}$ sec$^{-1}$ (Singh 1977; quoted, Mill 1985); surface photolysis half-life on a clean soft glass surface at 1.0 m from a GE Model RS sunlamp with half-life of 8400 minutes (Nestrick et al. 1980); solution photolysis in n-hexadecane with half-life of 56.8 minutes (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); reaction rate constant with OH radicals, $2 \times 10^{8}$ mole$^{-1}$ sec$^{-1}$ (Davenport et al. 1984; quoted, Mill 1985); half-lives: about 1 day in water, 0.1 day in vapor and 1-100 days in soil with 50 days for a small fraction in water column in equilibrium with sediment sorbed with TCDD (Mill 1985); atmospheric and aqueous photolysis half-life of 27 hours, based on measured rate constant for photolysis in a 90:10 mixture of distilled water and acetonitrile under summer sunlight (Dulin et al. 1986; quoted, Howard et al. 1991; Muto et al. 1991) and 81 hours after adjusting for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); half-life of aqueous dissolved TCDD in sunlight over four seasons at 40°N latitude is calculated to be: 118 hours in winter, 27 hours in spring, 21 hours in summer, 51 hours in fall and with rate constants: 0.14 day$^{-1}$ for winter, 0.61 day$^{-1}$ for spring, 0.78 day$^{-1}$ for summer, and 0.32 day$^{-1}$ for autumn (Podoll et al. 1986); photodegradation is a very rapid process at soil surface with a half-life of 10 minutes during the day (Facchetti et al. 1986); sunlight induced photolysis in isooctane with half-life of 14 minutes and dispersed as solid films with half-life of 300 hours (Buser 1988); first-order photolysis rate constant in isooctane was determined to be 0.15 minute$^{-1}$ and over 90% was lost in 21 minutes of irradiation in isooctane whereas only greater than 55% TCDD remained in soil after 15 days of irradiation (Kieatiwong et al. 1990); photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with half-life of 4.5 hours and 5.2 hours for native and $^{13}$C-labelled congeners in tetradeane solution, whereas half-lives for solid phase photolysis were relatively longer in fly ash (Tysklind & Rappe 1991); half-life of 31 minutes in hexadecane and 27 minutes in ethyl oleate (Dougherty et al. 1991); half-life from direct sunlight photolysis in water-acetonitrile in midday of mid-summer at 40°N was estimated to be 52 hours (quoted, Zeep 1991).

Oxidation: laboratory tests shown that 99.5% TCDD was oxidized in 21 seconds at 800°C while only 50% reacted at 700°C (Esposito et al. 1980; quoted, Crosby 1985); half-life for oxidation in vapor, about 13 days (Mill 1985); rate constant for reaction of OH radicals with aromatics are large, e.g. > $1 \times 10^{8}$ mole$^{-1}$
sec$^{-1}$, 1.7x$10^{13}$ molecul$e^{-1}$ cm$^3$ sec$^{-1}$; half-life in OH oxidation in the atmosphere is 200 hours, applied only to TCDD vapor (Podoll et al. 1986); room temperature gas-phase OH radical reaction rate constant was calculated to be 9x$10^{12}$ cm$^3$ molecul$e^{-1}$ sec$^{-1}$ corresponding to an atmospheric lifetime of about 3 days (Atkinson 1987a) and 8.0x$10^{12}$ cm$^3$ molecul$e^{-1}$ sec$^{-1}$ (Atkinson 1987b); photooxidation half-life of 22.3-223 hours, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987, quoted, Howard et al. 1991); the oxidative degradation of water dissolved TCDDs by ozone takes place only under alkaline conditions at pH 10 and 20°C, the reaction rate constant is 1.33x$10^7$ liter gram$^{-1}$ minute$^{-1}$ (Palauschek & Scholz 1987).

Hydrolysis: hydrolysis is not likely under environmental conditions (Callahan et al. 1979; Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aerobic half-life of 10032 hours, based on soil dieaway test data (Kearney et al. 1971; quoted, Howard et al. 1991) and 14160 hours, based on lake water and sediment dieaway test data (Ward & Matsumara 1978; quoted, Howard et al. 1991); half-life > 1.0 year (Callahan et al. 1979); anaerobic half-life of 40128-56640 hours, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation in water estimated to be 1x$10^{10}$ mL cell$^{-1}$ hour$^{-1}$ (Mabey et al. 1982).

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

- $k_1$: 6.30 mL gram$^{-1}$ hour$^{-1}$ (rainbow trout, calculated, Neely 1979)
- $k_1$: 4.64 mL gram$^{-1}$ hour$^{-1}$ (rainbow trout, experimental, Neely 1979)
- $k_2$: 2.12x$10^{4}$ hour$^{-1}$ (rainbow trout, calculated, Neely 1979)
- $k_2$: 5.00x$10^{4}$ hour$^{-1}$ (rainbow trout, experimental, Neely 1979)
- $k_1$: 108 mL gram$^{-1}$ day$^{-1}$ (rainbow trout, Branson et al. 1983, 1985; quoted, Adams et al. 1986; Sijm & Oppenhuizen 1988; Oppenhuizen & Sijm 1990)
- $k_2$: 0.012 day$^{-1}$ (rainbow trout, Branson et al. 1983, 1985; quoted, Adams et al. 1986; Sijm & Oppenhuizen 1988; Oppenhuizen & Sijm 1990)
- $k_1$: 476 mL gram$^{-1}$ day$^{-1}$ (fathead minnows, Adams et al. 1986)
- $k_2$: 0.120 day$^{-1}$ (fathead minnows, Adams et al. 1986)
- $k_1$: 1832, 1543, 1337, 1591 day$^{-1}$ (rainbow trout, exposed to 38 pg/L, 176 pg/L, 382 pg/L, 702 pg/L for 28 days, Mehrle et al. 1988; quoted, Oppenhuizen & Sijm 1990)
- $k_2$: 0.047, 0.041, 0.015, 0.043 day$^{-1}$ (rainbow trout, exposed to 38, 176, 382, 702 pg/L for 28 days, Mehrle et al. 1988; quoted, Oppenhuizen & Sijm 1990)
- $k_1$: 216, 604 L kg$^{-1}$ day$^{-1}$ (goldfish after 8 hours exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)
- $k_1$: 600 mL gram$^{-1}$ day$^{-1}$ (guppy, Oppenhuizen et al. 1986; quoted, Oppenhuizen & Sijm 1990)
\begin{align*}
\text{k}_2: & \quad 0.046 \text{ day}^{-1} \quad \text{(guppy, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990)} \\
\text{k}_2: & \quad 0.008 \text{ day}^{-1} \quad \text{(rainbow trout, quoted, Opperhuizen & Sijm 1990)} \\
\text{k}_1: & \quad 381 \text{ mL gram}^{-1} \text{ day}^{-1} \quad \text{(fathead minnows, quoted, Opperhuizen & Sijm 1990)} \\
\text{k}_2: & \quad 0.048 \text{ day}^{-1} \quad \text{(fathead minnows, quoted, Opperhuizen & Sijm 1990)} \\
\text{k}_1: & \quad 100 \text{ mL gram}^{-1} \text{ day}^{-1} \quad \text{(mosquito fish, quoted, Opperhuizen & Sijm 1990)}
\end{align*}
Common Name: 1,2,3,4,7-Pentachloro-dibenzo-p-dioxin
Synonym: 1,2,3,4,7-P,CDD
Chemical Name: 1,2,3,4,7-pentachloro-dibenzo-p-dioxin
CAS Registry No: 39227-61-7
Molecular Formula: ClC₆H₃OC₆Cl₄
Molecular Weight: 356.4

Melting Point (°C):
196 (quoted, Shiu et al. 1988)
188 (Friesen & Webster 1990)

Boiling Point (°C):
464.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
296.5 (LeBas method, Shiu et al. 1988)
146.22 (calculated as per Pearlman 1986, De Voogt et al. 1990)
142.92 (calculated as per Govers & De Voogt 1989, De Voogt et al. 1990)
197.74 (calculated-liquid density, Govers et al. 1990)

Molecular Volume (Å³):
224 (Friesen & Webster 1990)

Total Surface Area, TSA (Å²):
309 (Friesen & Webster 1990)

Heat of Fusion, ΔHₘₑₜ, kcal/mol:
6.214 (Friesen & Webster 1990)

Entropy of Fusion, ΔSₘₑₜ, cal/mol K (e.u.):

Fugacity Ratio at 25 °C (assuming ΔS = 13.5 e.u.), F:
0.0204 (Shiu et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C):
0.000018, 0.0000855 (20°C, ¹⁴C-labeled, gen. col.-HPLC/LSC, calculated, Friesen et al. 1985; quoted, Shiu et al. 1988)
0.0000955 (20°C, ¹⁴C labeled, gen. col.-HPLC/LSC, Webster et al. 1986)
Vapor Pressure (Pa at 25°C):
- \(8.8 \times 10^{-5}\) (calculated, Rordorf 1985a, b, 1987, 1989)
- \(1.0 \times 10^{-6}\) (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
- \(1.0 \times 10^{-6}\) (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

Henry's Law Constant (Pa m³/mol):
- 0.264 (calculated-P/C, Shiu et al. 1988)

Octanol/Water Partition Coefficient, log \(K_{ow}\):
- 9.44, 9.62, 10.02; 9.39, 9.65, 10.05 (HPLC-RT, linear; quadratic regressions, Sarna et al. 1984)
- 9.48, 8.80; 9.40, 8.64 (HPLC-RT, linear; quadratic regressions, Webster et al. 1985; quoted, Sijm et al. 1989a)
- 9.65, 7.44 (HPLC-RT, Burkhard & Kuehl 1986)
- 7.44 (quoted, De Voogt et al. 1990)
- 6.60 (slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)

Bioconcentration Factor, log \(B_{CF}\):
- 3.16 (fathead minnows, steady-state, wet weight, Muir et al. 1985, quoted, Adams et al. 1986)
- 2.91 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
- 3.16, 2.91 (fathead minnows, rainbow trout, De Voogt et al. 1990)
- 3.50, 4.50 (fathead minnows, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)

Sorption Partition Coefficient, log \(K_{oc}\):
- 4.85, 5.80, 6.38 (20°C, fulvic acid, humic acid, Aldrich humic acid, Webster et al. 1986b)
- 5.02 (DOC, De Voogt et al. 1990)
Half-Lives in the Environment:

Air: photodegradation half-life in a rotary photo-reactor adsorbed to clean silica gel by filtered < 290 nm of light, 92 hours (Koester & Hites 1992).

Surface water: under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile solution (4:6, v/v): half-life of 18.29 days in spring with rate constant of $0.466 \times 10^6$ sec$^{-1}$, 15.16 days in summer with rate constant of $0.562 \times 10^6$ sec$^{-1}$, 28.59 days in fall with rate constant of $0.298 \times 10^6$ sec$^{-1}$, 52.37 days in winter with rate constant of $0.163 \times 10^6$ sec$^{-1}$, and 76.82 days averaged over full year with rate constant of $0.111 \times 10^6$ sec$^{-1}$ (Choudhry & Webster 1985a, 1986); photolysis in water-acetonitrile (2:3, v/v) at 313 nm with half-life of 45.86 hours and the calculated midday, midseason direct phototransformation half-lives near water bodies at 40°N latitude: 18.4 days in spring, 15 days in summer, 29 days in fall and 52 days in winter (Choudhry & Webster 1989); 27 days in sunlit surface water and 0.94 days in surface water of actual pond (Friesen et al. 1990).

Groundwater:

Sediment:

Soil:

Biota: 3.1 days in fathead minnows (Adams et al. 1986); 2 days in whole body of rainbow trout (Muir & Yarechewski 1988; quoted, Muir et al. 1990)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis: rate constant of $4.31 \times 10^6$ sec$^{-1}$ in water-acetonitrile (2:3, v/v) at 313 nm and calculated half-lives under conditions of variable sunlight intensity at 40°N latitude: 18.29 days in spring with rate constant of $0.466 \times 10^6$ sec$^{-1}$, 15.16 days in summer with rate constant of $0.562 \times 10^6$ sec$^{-1}$, 28.59 days in fall with rate constant of $0.298 \times 10^6$ sec$^{-1}$, 52.37 days in winter with rate constant of $0.163 \times 10^6$ sec$^{-1}$, and 76.82 days averaged over full year with rate constant of $0.111 \times 10^6$ sec$^{-1}$ (Choudhry & Webster 1985a, 1986); rate constant of $4.315 \times 10^6$ sec$^{-1}$ in water-acetonitrile (3:3 v/v) at 313 nm (Choudhry & Webster 1985b); photolysis rate constant of $4.31 \times 10^6$ sec$^{-1}$ with a half-life of 45.86 hours 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: 4.03x10$^2$ day$^{-1}$ in spring, 4.86x10$^2$ day$^{-1}$ in summer, 2.58x10$^2$ day$^{-1}$ in fall, 1.41x10$^2$ day$^{-1}$ in winter with half-lives: 18 days in spring, 15 days in summer, 29 days in fall and 52 days in winter (Choudhry & Webster 1989); rate constant of 0.74 day$^{-1}$ under mid-summer sunlight at 50°N latitude in filtered-sterilized natural water and 0.058 day$^{-1}$ in (2:3, v/v) distilled water-acetonitrile (Friesen et al. 1990); photolytic half-life of 38 hours in fly-ash extract (Tysklind & Rappe 1991); half-life of 92 hours for photodegradation in
a rotary photoreactor adsorbed to clean silica gel by filtered < 290 nm of light (Koester & Hites 1992).

Oxidation:
Hydrolysis:
Biodegradation:
Biotransformation: biotransformation rate constant of 0.014 day⁻¹ for rainbow trout (Sijm et al. 1990).

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

\[ k₁: \quad 285 \text{ day}^{-1} \quad (\text{fathead minnows, Muir et al. 1985; quoted, Adams et al. 1986}) \]
\[ k₂: \quad 0.22 \text{ day}^{-1} \quad (\text{fathead minnows, Muir et al. 1985, quoted, Adams et al. 1986}) \]
\[ k₁: \quad 204 \text{ day}^{-1} \quad (\text{rainbow trout, Muir et al. 1985; quoted, Sijm et al. 1990}) \]
\[ k₂: \quad 0.28 \text{ day}^{-1} \quad (\text{rainbow trout, Muir et al. 1985; quoted, Sijm et al. 1990}) \]
\[ k₂: \quad 2.5 \times 10^2, 3.9 \times 10^2 \text{ day}^{-1} \quad (\text{rainbow trout for 2 to 21 days exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1990}) \]
Common Name: 1,2,3,4,7,8-Hexachloro-dibenzo-p-dioxin
Synonym: 1,2,3,4,7,8-H_{6}CDD
Chemical Name: 1,2,3,4,7,8-hexachloro-dibenzo-p-dioxin
CAS Registry No: 39227-26-8
Molecular Formula: Cl_{2}C_{6}H_{2}OC_{6}Cl_{4}
Molecular Weight: 391.0

Melting Point (°C):
273 (quoted, Shiu et al. 1988)
259-261 (quoted, Friesen et al. 1985)

Boiling Point (°C):
487.7 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):
317.4 (LeBas method, Shiu et al. 1988)
155.38 (calculated as per Pearlman 1986, De Voogt et al. 1990)
151.44 (calculated as per Govers & De Voogt 1989, De Voogt et al. 1990)
1.686 (intrinsic V/100, Hawker 1990)
206.96 (calculated-liquid density, Govers et al. 1990)

Molar Volume (cm³/mol):
Friesen & Webster 1990)

Molecular Volume (Å³): 239 (Friesen & Webster 1990)

Total Surface Area, TSA (Å²):
321 (Friesen & Webster 1990)

Heat of Fusion, ΔH_{fm}, kcal/mol:
7.22 (Friesen & Webster 1990)

Entropy of Fusion, ΔS_{fm}, cal/mol K (e.u.):
21.03 (Rordorf 1987,1989)

Fugacity Ratio at 25 °C (assuming ΔS = 13.5 e.u.), F:
0.00352 (Shiu et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C):
0.00000442; 0.0000161 (20°C, ¹⁴C-labeled, gen. col.-HPLC/LSC; calculated, Friesen et al. 1985; quoted, Shiu et al. 1988)
0.0000057 (20°C, ¹⁴C-labeled, gen. col.-HPLC/LSC, Webster et al. 1986b)
0.00000442 (selected, Shiu et al. 1988)
0.0000040; 0.00000644 (21°C; 26 °C, gen. col.-HPLC/LSC, Friesen & Webster 1990)
0.0000044 (20°C, quoted, De Voogt et al. 1990)
0.000004 (quoted, Paterson et al. 1990)

Vapor Pressure (Pa at 25°C):
5.10x10⁻⁹ (calculated, Rordorf 1985a,b, 1987,1989; quoted, Shiu et al. 1988)
3.20x10⁻⁷ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
3.96x10⁻⁴ (subcooled liquid value, GC-RT, Eitzer & Hites 1988)
7.85x10⁻⁶ (subcooled liquid, GC/Ms, Eitzer & Hites 1988)
5.10x10⁻⁹ (quoted, Paterson et al. 1990)
1.00x10⁻⁸ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

Henry's Law Constant (Pa m³/mol):
4.52 (calculated-P/C, Shiu et al. 1988)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:
10.36, 10.39, 10.89; 10.22, 10.44, 10.89 (HPLC-RT, linear; quadratic regressions, Sarna et al. 1984)
10.44, 7.79 (HPLC-RT, Burkhard & Kuehl 1986)
7.79 (quoted, De Voogt et al. 1990)
8.00 (quoted, Hawker 1990)
7.30 (calculated, Broman et al. 1991)
9.53 (quoted, HPLC-RT, Chessells et al. 1991)
9.53, 9.13 (mean lit. value, calculated-f const., Chessells et al. 1991)

Bioconcentration Factor, log BCF:
3.36 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
3.63 (fathead minnows, steady-state, wet weight, Muir et al. 1985, quoted, Adams et al. 1986)
3.36, 3.63 (rainbow trout, minnows, quoted, De Vrogt et al. 1990)
4.00, 5.00 (fathead minnows, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
3.36, 3.63 (quoted, Hawker 1990)

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3.41, 3.76 (fathead minnows, quoted, Opperhuizen & Sijm 1990)
3.45, 3.23 (rainbow trout, quoted, Opperhuizen & Sijm 1990)

Sorption Partition Coefficient, log $K_{oc}$:
5.41, 6.02, 6.22 (20°C, fulvic acid, humic acid, Aldrich humic acid, Webster et al. 1986b)
5.02 (DOC, De Voogt et al. 1990)
7.10 (calculated, Broman et al. 1991)

Half-Lives in the Environment:
Air: estimated reaction rate constant, 0.005 hour$^{-1}$ (Paterson et al. 1990); photodegradation in a rotary photoreactor adsorbed to clean silica gel by filtered < 290 nm of light, 140 hours (Koester & Hites 1992).
Surface water: under conditions of variable sunlight intensity at 40°N latitude: 7.57 days in spring with rate constant of $1.06 \times 10^6$ sec$^{-1}$, 6.27 days in summer with rate constant of $1.28 \times 10^6$ sec$^{-1}$, 11.87 days in fall with rate constant of $0.676 \times 10^6$ sec$^{-1}$, 21.57 days in winter with rate constant of $0.37 \times 10^6$ sec$^{-1}$, and 76.82 days averaged over full year with rate constant of $0.252 \times 10^6$ sec$^{-1}$ (Choudhry Webster 1985a, 1986); photolysis half-life of 24.5 hours 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 days in spring, 6.3 days in summer, 12.0 days in fall and 22.0 days in winter (Choudhry & Webster 1989); 81 days in sunlit surface water and 2.5 days in surface water of actual pond (Friesen et al. 1990); estimated reaction rate constant, 0.002 hour$^{-1}$ (Paterson et al. 1990).
Groundwater:
Sediment: estimated reaction rate constant to be $4.0 \times 10^6$ hour$^{-1}$ (Paterson et al. 1990).
Soil: estimated reaction rate constant to be $2.8 \times 10^6$ hour$^{-1}$ (Paterson et al. 1990).
Biota: 43 days in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990)

Environmental Fate Rate Constants or Half-Lives:
Volatilization:
Photolysis: calculated rate constants under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile (4:6 v/v) solution: $1.06 \times 10^6$ sec$^{-1}$ for spring with half-life of 7.57 days, $1.28 \times 10^6$ sec$^{-1}$ for summer with half-life of 6.27 days, $0.676 \times 10^6$ sec$^{-1}$ for fall with half-life of 11.87 days, $0.37 \times 10^6$ sec$^{-1}$ for winter with half-life of 21.57 days and $0.252 \times 10^6$ sec$^{-1}$ averaged over full year with half-life of 31.85 days (Choudhry & Webster 1985a, 1985c, 1986); $7.86 \times 10^6$ sec$^{-1}$ in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhry & Webster 1985a, 1985c, 1986)
1985b); photolysis rate constant of $7.86 \times 10^4$ sec$^{-1}$ with a half-life of 24.5 hours 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: $9.16 \times 10^2$ day$^{-1}$ for spring, $11.06 \times 10^2$ day$^{-1}$ for summer, $5.84 \times 10^2$ day$^{-1}$ for fall, $3.21 \times 10^2$ day$^{-1}$ for winter and with half-lives: 7.6 days in spring, 6.3 days in summer, 12.0 days in fall and 22.0 days in winter (Choudhry & Webster 1989); 0.28 day$^{-1}$ in natural water and 0.019 day$^{-1}$ in distilled water-acetonitrile (Friesen et al. 1990); photolytic half-life in the fly ash extract in tetradecane calculated to be 38 hours (Tysklind & Rappe 1991); photodegradation half-life in a rotary photoreactor absorbed to silica gel by filtered < 290 nm of light, 140 hours (Koester & Hites 1992).

Hydrolysis:

Oxidation: oxidative degradation rate constant of water dissolved PCDD is $5.02 \times 10^4$ liter gram$^{-1}$ minute$^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987).

Biodegradation:

Biotransformation:

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

$k_1$: 102 day$^{-1}$ (rainbow trout, Muir et al. 1985; quoted, Opperhuizen & Sijm 1990)

$k_2$: 0.046 day$^{-1}$ (rainbow trout, Muir et al. 1985; quoted, Opperhuizen & Sijm 1990)

$k_1$: 112 day$^{-1}$ (fathead minnows, Muir et al. 1985; quoted, Opperhuizen & Sijm 1990)

$k_2$: 0.030 day$^{-1}$ (fathead minnows, Muir et al. 1985; quoted, Opperhuizen & Sijm 1990)

$k_2$: 0.015 day$^{-1}$ (rainbow trout, quoted, Opperhuizen & Sijm 1990)

$k_2$: 0.0066 day$^{-1}$ (fathead minnows, quoted, Opperhuizen & Sijm 1990)
Common Name: 1,2,3,4,6,7,8-Heptachloro-dibenzo-p-dioxin
Synonym: 1,2,3,4,6,7,8-H\textsubscript{7}CDD
Chemical Name: 1,2,3,4,6,7,8-heptachloro-dibenzo-p-dioxin
CAS Registry No: 35822-46-9
Molecular Formula: Cl\textsubscript{3}C\textsubscript{6}HOC\textsubscript{6}Cl\textsubscript{4}
Molecular Weight: 425.2

Melting Point (°C):
265  (quoted, Shiu et al. 1988)

Boiling Point (°C):
507.2  (Rordorf 1987, 1989)

Density (g/cm\textsuperscript{3} at 20°C):
Molar Volume (cm\textsuperscript{3}/mol):
338.3  (LeBas method, Shiu et al. 1988)
164.52  (calculated as per Pearlman 1986, De Voogt et al. 1990)
159.96  (calculated as per Govers & De Voogt 1989, De Voogt et al. 1990)
1.778  (intrinsic \( V_i/100 \), Hawker 1990)
218.32  (calculated-liq. density, Govers et al. 1990)

Molar Volume (Å\textsuperscript{3}): 253  (Friesen & Webster 1990)
Total Surface Area, TSA (Å\textsuperscript{2}): 338  (Friesen & Webster 1990)
Heat of Fusion, \( \Delta H_{ fus} \), kcal/mol: 7.27  (Friesen & Webster 1990)
Entropy of Fusion, \( \Delta S_{ fus} \), cal/mol K (e.u.):
23.90  (Rordorf 1987, 1989)

Fugacity Ratio at 25 °C (assuming \( \Delta S = 13.5 \) e.u.), \( F \):
0.00423  (Shiu et al. 1988)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
0.0000024, 0.00000242  (20°C, \textsuperscript{14}C-labeled, gen. col.-HPLC/LSC; calculated, Friesen et al. 1985; quoted, Shiu et al. 1988)
0.0000024  (selected, Shiu et al. 1988)
0.000561, 0.000848  (quoted, calculated-\( \chi \), Nirmalakhanden & Speece 1989)
0.0000023; 0.00000256  (21°C; 26 °C, gen. col.-HPLC/LSC, Friesen & Webster 1990)
0.0000024  (20°C, quoted, De Voogt et al. 1990)
0.000002  (quoted, calculated-QSAR, Fiedler & Schramm 1990)
Vapor Pressure (Pa at 25°C):
- 7.5x10^{-10} (calculated, Rordorf 1985a,b, 1987,1989; quoted, Shiu et al. 1988)
- 3.2x10^{-8} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
- 1.024x10^{-6} (subcooled liquid value, GC-RT, Eitzer & Hites 1988)
- 1.93x10^{-6} (subcooled liquid, GC/MS, Eitzer & Hites 1988)
- 3.2x10^{-9} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

Henry's Law Constant (Pa m^3/mol):
- 0.133 (calculated-P/C, Shiu et al. 1988)

Octanol/Water Partition Coefficient, log \text{K}_{ow}:
- 11.29, 11.42, 11.90; 11.03, 11.50, 11.98 (HPLC-RT, linear; quadratic regressions, Sarna et al. 1984)
- 11.05, 11.50 (HPLC-RT, Sarna et al. 1984; quoted, Shiu et al. 1988)
- 11.38, 10.55; 11.05, 9.69 (HPLC-RT, linear; quadratic regressions, Webster et al. 1985; quoted, Sijm et al. 1989a)
- 8.20 (HPLC-RT, Burkhard & Kuehl 1986; quoted, Shiu et al. 1988)
- 8.20 (quoted, De Voogt et al. 1990)
- 7.92 (slow stirring-GC/MSD, from extract of fly ash, Sijm et al. 1989a)
- 9.86, 8.00 (calculated-QSAR, quoted, Fiedler & Schramm 1990)
- 8.00 (quoted, Hawker 1990)
- 8.00 (calculated, Broman et al. 1991)
- 10.52 (quoted, HPLC-RT, Chessells et al. 1991)
- 10.32, 9.85 (mean lit. value, calculated-f const., Chessells et al. 1991)

Bioconcentration Factor, log \text{BCF}:
- 2.71 (fathead minnows, steady-state, wet weight, Muir et al. 1985, quoted, Adams et al. 1986)
- 3.15 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
- 2.71, 3.15 (fathead minnows, rainbow trout, quoted, De Voogt et al. 1990)
- 3.32, 4.32 (fathead minnows, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
- 2.71, 3.15 (quoted, Hawker 1990)
- 2.70, 2.70 (fathead minnows, quoted, Opperhuizen & Sijm 1990)
- 3.23, 3.04 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
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 (calculated, Broman et al. 1991)

Half-Lives in the Environment:

Air:
- Surface water: 11 hours in n-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhry & Webster 1982); solution photolysis half-life at 1.0 m from a GE Model sunlamp, 30 hours (Nestrick et al. 1980); photolysis half-life of 30 hours in n-hexadecane solution (Mamantov 1984); direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: spring, 56.46 days; summer, 47.33 days; fall, 87.86 days; winter, 155.79 days and averaged over full year, 2393 days (Choudhry & Webster 1985b, 1986); photolysis half-life of 190.97 hours 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: 57 days in spring, 47 days in summer, 88 days in fall and 156 days in winter (Choudhry & Webster 1989); half-life of 81 days in sunlit filtered and sterilized surface water and 2.5 days in surface water of actual pond at 50°N latitude (Friesen et al. 1990); 53.4 and 32.6 hours in native and 13C-labelled congeners respectively in extract from fly ash (Tysklind & Rappe 1991).

Groundwater:

Sediment:

Soil:

Biota: 17.2 days in fathead minnows (Adams et al. 1986); >336 days in carp (Kuehl et al. 1987); 39 days in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990); 27.2 days in lactating cows (Olling et al. 1991).

Environmental Fate Rate Constants or Half-Lives:

Volatileization:

Photolysis: 11 hours in n-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhry & Webster 1982); solution photolysis half-life at 1.0 m from a GE Model sunlamp, 30 hours and surface photolysis half-life on clean soft glass surface under the same conditions, 52.3 hours (Nestrick et al. 1980); 30 hours in n-hexadecane solution (Mamantov 1984); first order rate constant of $1.02 \times 10^6$ sec$^{-1}$ 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: spring, 56.46 days; summer, 47.33 days; fall, 87.86 days; winter, 155.79 days and averaged over full year, 2392.68 days (Choudhry & Webster 1985b, 1986); photolysis rate constant of $1.02 \times 10^6$ sec$^{-1}$.
with a half-life of 190.97 hours 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: 1.24x10^2 day^-1 for spring, 1.48x10^2 day^-1 for summer, 0.80x10^2 day^-1 for fall, 0.45x10^2 day^-1 for winter with half-lives: 57 days in spring, 47 days in summer, 88 days in fall and 156 days in winter (Choudhry & Webster 1989); sunlight photolysis rate constant of 0.28 day^-1 in filtered and sterilized natural water and 0.019 day^-1 in (2:32, v/v) distilled water-acetonitrile solution at 50°N (Friesen et al. 1990); half-lives of 53.4 and 32.6 hours in native and 13C-labelled congeners respectively in extract from fly ash (Tysklind & Rappe 1991).

Oxidation: oxidative degradation rate constant of water dissolved PCDD by ozone is 5.46x10^4 liter gram^-1 minute^-1 under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987).

Hydrolysis:

Biodegradation:

Biotransformation:

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

\[k_1: \begin{align*}
56 & \text{ day}^{-1} \quad \text{(rainbow trout, Muir et al. 1985; quoted, Opperhuizen \\ & Sijm 1990)} \\
0.042 & \text{ day}^{-1} \quad \text{(rainbow trout, Muir et al. 1985; quoted, Opperhuizen \\ & Sijm 1990)}
\end{align*}\]

\[k_2: \begin{align*}
19 & \text{ day}^{-1} \quad \text{(fathead minnows, Muir et al. 1985; quoted, Adams et al. \\ & 1986; Opperhuizen & Sijm 1990)} \\
0.040 & \text{ day}^{-1} \quad \text{(fathead minnows, Muir et al. 1985; quoted, Adams et al. \\ & 1986; Opperhuizen & Sijm 1990)} \\
0.0092 & \text{ day}^{-1} \quad \text{(fathead minnows, quoted, Opperhuizen & Sijm 1990)} \\
0.0110 & \text{ day}^{-1} \quad \text{(rainbow trout, quoted, Opperhuizen & Sijm 1990)}
\end{align*}\]
Common Name: Octachloro-dibenzo-p-dioxin
Synonym: O₈CDD, OCDD
Chemical Name: octachloro-dibenzo-p-dioxin
CAS Registry No: 3268-87-9
Molecular Formula: Cl₈C₆OC₆Cl₄
Molecular Weight: 460.0

Melting Point (°C):
318-326 (quoted lit., Pohland & Yang 1972)
332 (quoted, Shiu et al. 1988)
325-326 (quoted, Friesen et al. 1985; Shiu et al. 1987)
Boiling Point (°C):
510 (Rordorf 1987, 1989)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
359.2 (LeBas method, Shiu et al. 1987, 1988)
173.66 (calculated as per Pearlman 1986, De Voogt et al. 1990)
168.48 (calculated as per Govers & De Voogt 1989, De Voogt et al. 1990)
1.868 (intrinsic V/100, Hawker 1990)
229.6, 229.11 (calculated-liq. density, crystalline volume, Govers et al. 1990)
Molecular Volume (Å³):
Total Surface Area, TSA (Å²):
314.90 (Doucette & Andren 1987, 1988b)
Entropy of Fusion, ΔSₘₑₜ, cal/mol K (e.u.):
Fugacity Ratio at 25 °C (assuming ΔS = 13.5 e.u.), F:
0.00107 (Shiu et al. 1987)
0.00115 (Shiu et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C):
2.0x10⁻⁶ (Barrie et al. 1983)
4.0x10⁻⁷ (¹⁴C-labelled, gen. col.-HPLC/LSC, Webster et al. 1983; quoted, Shiu et al. 1988)
4.0 \times 10^{-7}, 3.17 \times 10^{-7} \ (20^\circ C, \ ^{14}C\text{-labeled, gen. col.-HPLC/LSC, calculated, Friesen et al. 1985})

4.0 \times 10^{-7} \ (20^\circ C, \ ^{14}C\text{-labelled, gen. col.-HPLC/LSC, Webster et al. 1985})

1.8 \times 10^{-4} \ \text{(Opperhuizen 1986)}

7.36 \times 10^{-6} \ \text{(gen. col.-HPLC/UV, Shiu et al. 1987)}

1.0 \times 10^{-7} \ \text{(^{14}C\text{-labeled-LSC, Srinivasan & Fogler 1987)}}

7.4 \times 10^{-8} \ \text{(gen. col.-GC/ECD, Shiu et al. 1988)}

7.4 \times 10^{-8} \ \text{(extrapolated, gen. col.-GC/ECD, Doucette & Andren 1988a)}

4.0 \times 10^{-7} \ \text{(20^\circ C, quoted, De Voogt et al. 1990)}

7.36 \times 10^{-7} \ \text{(quoted, Paterson et al. 1990)}

4.01 \times 10^{-7} - 7.46 \times 10^{-4}; 2.90 \times 10^{-7} \ \text{ (quoted; calculated-QSAR, Fiedler & Schramm 1990)}

7.0 \times 10^{-8} \ \text{(quoted, Gobas & Schrap 1990)}

6.44 \times 10^{-5} \ \text{(quoted, Servos et al. 1992a)}

\text{Vapor Pressure (Pa at 25^\circ C):}

2.40 \times 10^{-5}, 1.8 \times 10^{-5} \ \text{ (quoted, calculated-volatilization rate, Dobbs & Cull 1982)}

2.40 \times 10^{-5} \ \text{ (quoted, Cull et al. 1983)}

8.70 \times 10^{-6} \ \text{ (20^\circ C, gas saturation, Webster et al. 1985; quoted, Shiu et al. 1988)}

1.10 \times 10^{-10} \ \text{ (calculated, Rordorf 1985a,b, 1986a,b, 1987,1989; quoted, Shiu et al. 1987,1988)}

2.51 \times 10^{-10} \ \text{ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf 1986)}

2.77 \times 10^{-7} \ \text{ (subcooled liquid value, GC-RT, Eitzer & Hites 1988)}

1.10 \times 10^{-10} \ \text{ (quoted, Paterson et al. 1990)}

2.72 \times 10^{-7} \ \text{ (subcooled liquid value, GC-RT, Eitzer & Hites 1989)}

1.60 \times 10^{-10} \ \text{ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substituted no. plot, Rordorf et al. 1990)}

1.2 \times 10^{-7} \ \text{ (quoted, Servos et al. 1992a)}

\text{Henry’s Law Constant (Pa m}^3/\text{mol):}

0.683 \ \text{(calculated-P/C, Shiu et al. 1987,1988)}

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

8.31 \ \text{(Garten & Trabka 1983)}

8.50 \ \text{(Bruggeman et al. 1984; quoted, Opperhuizen 1986)}

12.21, 12.60, 12.97; 11.82, 12.72, 13.08 \ \text{ (HPLC-RT, linear; quadratic regressions, Sarna et al. 1984)}

10.56, 7.53 \ \text{(calculated, Doucette 1985; quoted, Shiu et al. 1988)}

11.16, 12.72 \ \text{ (HPLC-RT, Sarna et al. 1984; quoted, Shiu et al. 1988)}
12.26, 11.35; 11.76, 10.07 (HPLC-RT, linear; quadratic regressions, Webster et al. 1985; quoted, Sijm et al. 1989a)
8.60 (HPLC-RT, Burkhard & Kuehl 1986; quoted, Geyer et al. 1987; Shiu et al. 1988)
7.59, 10.56, 7.33 (gen. col.-GC/ECD, calculated-f-const., TSA, Doucette & Andren 1987)
7.59 (quoted, Geyer et al. 1987)
8.40 (quoted, Gobas et al., 1987)
7.59-8.60 (selected, Shiu et al. 1987)
7.59, 10.56, 10.09, 7.83, 7.65, 7.53, 7.46 (selected exp. value, calculated-π const., f-const, HPLC-RT, MW, -x, TSA, Doucette and Andren 1988b)
8.20 (selected, Shiu et al. 1988; quoted, Gobas et al. 1988; Sijm et al. 1989a; Friedler & Schramm 1990; Gobas et al., 1990; Gobas & Schrap 1990; Hawker 1990; Paterson et al. 1990; Loonen et al. 1991; Servos et al. 1992a,b)
7.59 (gen. col.-GC, Shiu et al. 1988)
8.60 (quoted, De Voogt et al. 1990)
10.56 (calculated-QSAR, Fiedler & Schramm 1990)
8.20 (quoted, Hawker 1990)
8.20 (calculated, Broman et al. 1991)
7.59, 10.96 (quoted values: gen. col. method, HPLC-RT, Chessells et al. 1991)
10.28, 10.56 (mean lit. value, calculated-f const., Chessells et al. 1991)

Bioconcentration Factor, log BCF:
-1.10 (rodents, Garten & Trabalka 1983)
3.35 (fathead minnows, steady-state, wet weight, Muir et al. 1985,1986; quoted, Adams et al. 1986)
1.93 (rainbow trout, steady-state, wet weight, Muir et al. 1985,1986)
1.93, 3.35 (trout fry, fathead minnows, 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. based, Geyer et al. 1987)
1.90, 3.10 (guppy: in whole fish, in lipid, Gobas et al. 1987)
6.33 (plant parts, calculated-vapor pressure, Reischl et al. 1989)
5.85 (plant parts, calculated-vapor pressure & HLC, Reischl et al. 1989)
3.35, 1.93 (fathead minnows, rainbow trout, quoted, De Voogt et al. 1990)
3.35, 1.93 (quoted, Hawker 1990)
2.85, 3.97 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
4.35, 5.35 (fathead minnows, quoted, Gobas & Schrap 1990)
3.93, 4.93 (rainbow trout, quoted, Gobas & Schrap 1990)
2.15, 1.49 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
3.34 (fathead minnows, quoted, Opperhuizen & Sijm 1990)
2.85 (predicted for biota held in lake enclosures exposed to water concentration of 0.1 ng/g for 0-10 days, Servos et al. 1992b)
2.15 (caged invertebrates exposed to water concn. 2.0 ng/L for 0-10 days, Servos et al. 1992b)
2.32 (caged unionid clams exposed to water concn. 2.9 ng/L for 0-10 days, Servos et al. 1992b)
2.32 (caged white suckers gill exposed to water concn. 2.9 ng/L for 0-10 days, Servos et al. 1992b)
1.89 (caged white suckers carcass exposed to water concn. 1.1 ng/L for 0-10 days, Servos et al. 1992b)
2.42 (caged invertebrates exposed to water concn. 0.6 ng/L for 14-24 days, Servos et al. 1992b)
2.34 (caged unionid clams exposed to water concn. 0.5 ng/L for 14-24 days, Servos et al. 1992b)
2.75 (caged white suckers gill exposed to water concn. 1.3 ng/L for 14-24 days, Servos et al. 1992b)
2.24 (caged white suckers carcass exposed to water concn. 0.4 ng/L for 14-24 days, Servos et al. 1992b)
3.97 (caged white suckers gill exposed to water concn. 2.8 ng/L for 0-104 days, Servos et al. 1992b)
3.95 (caged white suckers carcass exposed to water concn. 2.7 ng/L for 0-104 days, Servos et al. 1992b)

Sorption Partition Coefficient, log $K_{oc}$:
7.08 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
5.92 (DOC, De Voogt et al. 1990)
7.90 (calculated, Broman et al. 1991)

Half-Lives in the Environment:
Air: estimated reaction rate constant, 0.0015 hour$^{-1}$ (Paterson et al. 1990);
photodegradation half-life in a rotary photo-reactor adsorbed to clean silica gels by filtered < 290 nm of light, 270 hours (Koester & Hites 1992).
Surface water: solution photolysis half-life at 1.0 m from a GE Model RS sunlamp, 24.3 hours (Nestrick et al. 1980); direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: spring, 20.53 days; summer, 17.85 days; fall, 31.26 days; winter, 50.45 days and averaged over full year, 863.22 days (Choudhry & Webster 1986); rate constant of $1.064 \times 10^6$ sec$^{-1}$ in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhry & Webster 1985a, 1986); photolysis half-life of 183.95 hours in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, midseason direct photolysis half-lives near water bodies at 40°N latitude: 21 days in spring, 18 days in summer, 31 days in fall and 50 days in winter (Choudhry & Webster 1989); half-life of 4.0 days in the water column of an experimental lake in northwestern Ontario (Servos et
al. 1989); calculated transformation rate constant in simulated lake enclosure, 1.6x10^3 hour^-1 (Servos et al. 1992a).

Groundwater:
Sediment: estimated reaction rate constant, 5x10^3 to 1.0x10^6 hour^-1 (Paterson et al. 1990); calculated half-life, 10 years with a transformation rate constant of 7.9x10^4 hour^-1 (Servos et al. 1992a).

Soil: undergoes photoreduction on soil surfaces to lower chlorinated congeners (Kieatiwong et al. 1990); estimated reaction rate constant, 7.0x10^7 hour^-1 (Paterson et al. 1990).

Biota: half-life of elimination from rat, 21 days (Norback et al. 1975; quoted, Birbaum 1985); elimination half-life of 13.9 days for fathead minnows (Muir et al. 1985, Adams et al. 1986); elimination half-life of 5-13 days for both rainbow trout and fathead minnows (Muir et al. 1986); mean biological half-life in rainbow trout, about 15 days (Niimi 1986); 15 days in rainbow trout (Niimi & Oliver 1986; quoted, Muir et al. 1986,1990).

Environmental Fate Rate Constants or Half-Lives:
Volatilization:
Photolysis: photolytic half-life by both natural sunlight and fluorescent black light in hexane solution, 16 hours (Dobbs & Grant 1979; quoted, Choudry & Webster 1982); solution photolysis half-life at 1.0 m from a GE Model RS sunlamp, 24.3 hours and surface photolysis on clean soft glass surface under the same condition is 815 hours (Nestrick et al. 1980); half-life photolysis in hexadecane solution, 24.3 hours (Mamantov 1984); first-order rate constant of photolysis in water acetonitrile (2:3, v/v) at 313 nm was 1.06x10^6 sec^-1 and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: spring, 20.53 days; summer, 17.85 days; fall, 31.26 days; winter, 50.45 days; and averaged over full year, 863.22 days (Choudhry & Webster 1986; quoted, Muto et al. 1991); photolysis rate constant of 1.06x10^6 sec^-1 with a half-life of 183.95 hours 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: 3.45x10^2 day^-1 for spring, 3.97x10^2 day^-1 for summer, 2.27x10^2 day^-1 for fall, 1.40x10^2 day^-1 for winter with half-lives: 21 days in spring, 18 days in summer, 31 days in fall and 50 days in winter (Choudhry & Webster 1989); calculated photolysis decay rate constants when irradiated with UV light at 254 nm for fly ash suspensions in distilled water, 1.77x10^5 sec^-1 and 4.62x10^5 sec^-1 for fly ash suspensions in water-acetonitrile solution (2:3, v/v) is 1.42x10^5 sec^-1 and for fly ash suspensions in water-acetonitrile solution (2:3, v/v) with ozone is 2.74x10^5 sec^-1 (Muto et al. 1991); photolytic half-lives in extract of fly ash and in tetradecane solution: 37.3 hours-native congener, 29.6 hours for 13C-labelled congener (Tysklind & Rappe 1991).
Oxidation: oxidative degradation rate of water dissolved OCDD by ozone is $1.51 \times 10^4$ liter gram$^{-1}$ minute$^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987).

Hydrolysis:
Biodegradation:
Biotransformation:

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

$k_1$: 142 day$^{-1}$ (fathead minnows, Muir et al. 1985; quoted, Adams et al. 1986)
$k_2$: 0.05 day$^{-1}$ (fathead minnows, Muir et al. 1985, quoted, Adams et al. 1986)
$k_1$: 11.0 day$^{-1}$ (rainbow trout, Muir et al. 1985)
$k_2$: 0.12 day$^{-1}$ (rainbow trout, Muir et al. 1985)
$k_1$: 5.0-17.0 day$^{-1}$ (rainbow trout, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)
$k_2$: 0.103-0.142 day$^{-1}$ (rainbow trout, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)
$k_1$: 142 day$^{-1}$ (fathead minnows, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)
$k_2$: 0.053 day$^{-1}$ (fathead minnows, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)
$k_1$: 984 day$^{-1}$ (guppy, Gobas & Schrap 1990)
$k_2$: 1.4 day$^{-1}$ (guppy, Gobas & Schrap 1990)
$k_2$: 0.046 day$^{-1}$ (rainbow trout, quoted, Opperhuizen & Sijm 1990)
$k_1$: 60 day$^{-1}$ (filter-feeder, Servos et al. 1992b)
$k_2$: 0.12 day$^{-1}$ (filter-feeder, Servos et al. 1992b)
$k_1$: 30 day$^{-1}$ (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)
$k_2$: 0.08 day$^{-1}$ (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)
4. Chlorinated Dibenzo-furans

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4.5 References .............................................. 561
4.1 List of Chemicals and Data Compilations
Common Name: Dibenzo furan
Synonym: diphenylene oxide
Chemical Name: dibenzofuran
CAS Registry No: 132-64-9
Molecular Formula: C$_4$H$_{10}$O
Molecular Weight: 168.21

Melting Point (°C):
86.7 (Weast 1982-83)
82. (Banerjee et al. 1980; Pearlman et al. 1984)
84-92 (Stephenson & Malanowski 1987)
86.5 (Rordorf 1986, 1989)

Boiling Point (°C): 287
287 (quoted, Weast 1982-83; Stephenson & Malanowski 1987)
273 (calculated, Rordorf 1986, 1989)

Density (g/cm$^3$ at 20°C):
1.0886 (99°C, Weast 1982-83)

Molar Volume (cm$^3$/mol):
226.4 (LeBas method)
154.4 (calculated-density, Stephenson & Malanowski 1987)

Molecular Volume (Å$^3$):
152.438 (Pearlman et al. 1984)

Total Surface Area, TSA (Å$^2$):
183.75 (Pearlman et al. 1984)
176.3 (Doucette & Andren 1987)

Heat of Fusion, $\Delta H_{fus}$, kcal/mol:
4.6845 (Rordorf 1989)

Entropy of Fusion, $\Delta S_{fus}$, cal/mol K (e.u.):
12.90 (Rordorf 1986, 1989)

Fugacity Ratio at 25 °C (assuming $\Delta S = 13.5$ e.u.):
0.246 (at M.P. = 86.5°C)

Water Solubility (g/m$^3$ or mg/L at 25°C):
3.11 (Lu et al. 1978; quoted, Pearlman et al. 1984)
10.03 (shake flask-HPLC/UV, Banerjee et al. 1980)
6.56  (selected average, Pearlman et al. 1984)
4.22  (gen. col.-GC, Doucette & Andren 1988a, quoted, Friesen et al. 1990)
1.00  (selected, Isnard & Lambert 1988 1989)
4.75  (gen. col.-HPLC/UV, Shiu & Mackay 1992)

Vapor Pressure (Pa at 25°C):
- 2.026  (extrapolated liquid value, Antoine eqn., Stephenson & Malanowski 1987)
- 0.35   (gas saturation, Rordorf 1986, 1989)
- 0.40   (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

Henry’s Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, log K_{ow}:
- 4.12  (Hansch & Leo 1979; quoted, Birnbaum 1985)
- 4.17  (shake flask-HPLC/UV, Banerjee et al. 1980)
- 4.12  (Veith et al. 1979; quoted, Mackay 1982)
- 3.91, 4.12, 4.18; 3.96, 4.10, 4.17 (HPLC-RT, linear regressions; quadratic regressions, Sarna et al. 1984)
- 3.92  (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
- 4.31  (gen. col.-GC/ECD, Doucette & Andren 1987)
- 4.12, 4.04 (calculated-f const., TSA, K_{ow}, Doucette & Andren 1987)
- 4.31, 4.12, 4.04, 3.86, 4.11, 4.57, 4.13 (selected exptl., calculated-π-const, f-const., HPLC-RT, MW, χ, TSA, Doucette & Andren 1988b)
- 4.33  (gen. col.-HPLC/UV, Shiu & Mackay 1992)

Bioconcentration Factor, log BCF:
- 3.13  (fathead minnow, 28 days exposure, Veith et al. 1979)
- 3.13, 2.80 (quoted exptl., calculated-K_{ow}, Mackay 1982)
- 3.13, 3.13 (quoted exptl., calculated-χ, Sabljic 1987)
- 3.13  (calculated-K_{ow}, Isnard & Lambert 1989)

Sorption Partition Coefficient, log K_{oc}:
Half-Lives in the Environment:

Air: 1.9-19 hours, based on estimated rate constants for reaction with hydroxyl radicals in air (Atkinson 1987b; Howard et al. 1991).

Surface water: 168-672 hours, based on aerobic acclimated and unacclimated groundwater die-away test data (Lee et al. 1984; quoted; Ward et al. 1986; Howard et al. 1991).


Sediment:

Soil: 168-672 hours, based on aerobic acclimated and unacclimated groundwater die-away test data (Lee et al. 1984; quoted, Ward et al. 1986; Howard et al. 1991).

Biota:

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation: gas phase reaction rate constant with OH radicals was calculated to be $3.4 \times 10^{11}$ cm$^3$ molecule$^{-1}$ sec$^{-1}$ corresponding to an atmospheric lifetime of about 8 hours (Atkinson 1987a) and $3.3 \times 10^{11}$ cm$^3$ molecule$^{-1}$ sec$^{-1}$ (Atkinson 1987b); photooxidation half-life was estimated to be between 1.9-19 hours, based on estimated rate constant with OH radicals in air (Atkinson 1987b; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: biodegradation half-life was estimated to be 168-672 hours and anaerobic half-life of 672-2688 hours, based on aerobic acclimated and unacclimated groundwater die-away test data (Lee et al. 1984; quoted, Ward et al. 1986; Howard et al. 1991); nonautoclaved groundwater samples at hazardous waste site with a concentration of approximate 0.09 mg/liter are degraded by microbes at rates about 30% per week while the levels of the controls decreased only about half that rate (Lee et al. 1984).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
Common Name: 2,8-Dichlorodibenzofuran
Synonym: 2,8-DCDF
Chemical Name: 2,8-dichlorodibenzofuran
CAS Registry No: 5409-83-6
Molecular Formula: C₆H₄OC₆H₂Cl₂
Molecular Weight: 237.1

Melting Point (°C):
184-185 (Kuroki et al. 1984; quoted, Rordorf 1989)
185 (Van den Berg et al. 1985)

Boiling Point (°C):
375 (calculated, Rordorf 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
226.4 (LeBas method)

Molecular Volume (Å³):

Total Surface Area, TSA (Å²):
212.8 (Doucette & Andren 1987)
216.56 (van der Waals surface area, Dunn III et al. 1986)

Heat of Fusion, ΔHₘ₀, kcal/mol:
5.60 (Rordorf 1989)

Entropy of Fusion, ΔSₘ₀, cal/mol K, (e.u.):
13.145 (Rordorf 1989)

Fugacity Ratio at 25 °C (assuming ΔS = 13.5 e.u.), F:
0.0268

Water Solubility (g/m³ or mg/L at 25°C):
0.0145 (gen. col.-GC, Doucette & Andren 1988a, quoted, Friesen et al. 1990)

Vapor Pressure (Pa at 25°C):
3.9x10⁻⁴ (calculated-B.P. and ΔHₘ₀, Rordorf 1989)

Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
5.56, 5.97, 6.16; 5.65, 5.95, 6.15 (HPLC-RT, linear regressions; quadratic regressions, 
Sarna et al. 1984)
5.30 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
5.44 (gen. col.-GC/ECD, Doucette & Andren 1987)
5.65, 4.91 (calculated-f const., calculated-TSA-\( K_{\text{OW}} \), Doucette & Andren 1987)
5.44, 5.65, 5.53, 5.12, 4.92, 5.42, 5.01 (selected exptl., calculated-\( \pi \)-const, f-const., 
HPLC-RT, MW, \( \chi \), TSA, Doucette & Andren 1988b)

Bioconcentration Factor, log BCF:

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

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: mean biological half-life in rainbow trout, about 12 days (Niimi 1986).

Environmental Fate Rate Constants or Half-Lives:
- Volatilization:
- Photolysis: when 5 mg/liter in methanol was irradiated by sunlight simulator more than 
  95% disappears within 48 hours while a similar experiment with highly purified 
  methanol solution reveals only very slow photolysis within the same period of 
  irradiation and results were same with 10 mg/liter in methanol solution (Crosby 
  & Moilanen 1973; quoted, Choudhry & Hutzinger 1982).
- Hydrolysis:
- Oxidation:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:
Common Name: 2,3,7,8-Tetrachlorodibenzofuran
Synonym: 2,3,7,8-TCDF
Chemical Name: 2,2,7,8-Tetrachlorodibenzofuran
CAS Registry No: 51207-31-9
Molecular Formula: C_{34}H_{2}Cl_{2}O_{2}C_{4}H_{2}Cl_{2}
Molecular Weight: 306

Melting Point (°C):
- 227-228 (Gray et al. 1976)
- 219-221 (Kuroki et al. 1984)
- 227-228 (quoted, Van den Berg et al. 1985)
- 227, 228 (quoted, Rordorf 1989)

Boiling Point (°C): 438.3 (calculated, Rordorf 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
- 268.2 (LeBas method)

Molecular Volume (Å³):

Total Surface Area, TSA (Å²):
- 247.73 (van der Waals surface area, Dunn III et al. 1986)
- 212.8 (Doucette & Andren 1987)

Heat of Fusion, ΔH_fus, kcal/mol:
- 8.748 (Rordorf 1989)

Entropy of Fusion, ΔS_fus, cal/mol K (e.u.):
- 17.447 (Rordorf 1989)

Fugacity Ratio at 25 °C (assuming ΔS = 13.5 e.u.), F:
- 0.0000251

Water Solubility (g/m³ or mg/L at 25°C):
- 0.000419 (22.7 °C, gen. col.-HPLC/LSC, Friesen et al. 1990; quoted, Mackay 1991)
- 0.000640 (quoted, Ma et al. 1990)
- 0.00351 (calculated-QSAR, Fiedler & Schramm 1990)
Vapor Pressure (Pa at 25°C):
2.0x10^-6 (quoted, Van den Berg et al. 1985)
0.000002 (correlated, Rordorf 1989)
0.0001228 (GC-RT, subcooled liquid value, Eitzer & Hites 1988)

Henry’s Law Constant (Pa m^3/mol):
1.50 (calculated for tetrachloro-PCDFs, Eitzer & Hites 1989)

Octanol/Water Partition Coefficient, log K_{ow}:
5.82 (HPLC-RT, Burkhard & Kuehl 1986)
6.53 (slow stirring, GC/MS, from mixture of fly ash extract, Sijm et al. 1989a)
6.19 (correlated, Ma et al. 1990)
7.10 (calculated-QSAR, Fiedler & Schramm 1990)
7.70 (calculated, Broman et al. 1991)

Bioconcentration Factor, log BCF:
4.82 (guppy, Opperhuizen et al. 1986)
3.78, 3.39 (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 days, Mehrle et al. 1988)
3.64, 3.41 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
3.82 (guppy, quoted, Opperhuizen & Sijm 1990)

Sorption Partition Coefficient, log K_{oc}:
5.20 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
7.50 (calculated, Broman et al. 1991)

Half-Lives in the Environment:
Air:
Surface water: 90 minutes in isooctane solution in summer sunlight (Palsuschek & Scholz 1987).
Groundwater:
Sediment:
Soil:
Biota: half-lives of elimination: from rat, 2 days (Birnbaum et al. 1980; quoted, Birnbaum 1985); 8 days from monkey (Birnbaum et al. 1981; quoted, Birnbaum 1985); 2-4 days from mouse (Decad et al. 1981b; quoted, Birnbaum 1985); 40 days from guinea pig (Decad et al. 1981a; Ioannou et al. 1983; quoted, Birnbaum 1985); elimination half-lives: in guinea pigs, 20 days; rats, < 2 days;
moneys, 8 days; and mice, 2-4 days (quoted, Van den Berg et al. 1985); half-life in carp, <336 days (Kuehl et al. 1987); elimination half-life of 3.0 days, 0.27 day (rainbow trout, exposed to 0.41 ng/L, 3.93 ng/L for 28 days, Mehrle et al. 1988); elimination half-life of 0.8 day for lactating cows (Olling et al. 1991).

Environmental Fate Rate Constants or Half-Lives:

Volatilization:
Photolysis: sunlight induced photolysis half-life, 220 minutes in isooctane solution, and solid phase photolysis half-life, 120 hours with PCDF dispersed as solid films (Buser 1988); photolytic half-life in extract of fly ash and in tetradeane solution: 9.8 hours for native congener and 3.0 hours for $^{13}$C-labelled congener (Tysklind & Rappe 1991).

Hydrolysis:
Oxidation: room temperature OH radical reaction rate constant calculated to be $2.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ sec$^{-1}$ (Atkinson 1987b); oxidative degradation rate constant for water dissolved PCDF by ozone is $1.32 \times 10^8$ liter gram$^{-1}$ minute$^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987).

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

- $k_1$: 400 day$^{-1}$ (guppy, exposed to fly ash extract, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990)
- $k_2$: 0.062 day$^{-1}$ (guppy, exposed to fly ash extract, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990)
- $k_1$: 1228, 6853 day$^{-1}$ (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 days, Mehrle et al. 1988; quoted, Opperhuizen & Sijm 1990)
- $k_2$: 0.28, 2.60 day$^{-1}$ (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 days, Mehrle et al. 1988; quoted, Opperhuizen & Sijm 1990)
Common Name: 2,3,4,7,8-Pentachlorodibenzofuran
Synonym: 2,3,4,7,8-PCDF
Chemical Name: 2,3,4,7,8-pentachlorodibenzofuran
CAS Registry No: 51207-31-4
Molecular Formula: C₂₆H₂₄Cl₆O₆HCl₃
Molecular Weight: 340.42

Melting Point (°C):
196-196.5 (Kuroki et al. 1984)
196, 196.5 (Rordorf 1989)

Boiling Point (°C):
464.7 (calculated, Rordorf 1989)

Density (g/cm³ at 20°C):
289.1 (LeBas method)

Molar Volume (cm³/mol):
262.71 (van der Waals surface area, Dunn III et al. 1988)

Heat of Fusion, ΔHₘₑₜ, kcal/mol:
75.05 (Rordorf 1989)

Entropy of Fusion, ΔSₘₑₜ, cal/mol K (e.u.):
21.51 (Rordorf 1989)

Fugacity Ratio at 25 °C (assuming ΔS = 13.5 e.u.):
0.001125

Water Solubility (g/m³ or mg/L at 25°C):
0.000515 (calculated-QSAR, Fiedler & Schramm 1990)
0.000236 (22.7°C, gen. col.-GC/MS, Friesen et al. 1990)

Vapor Pressure (Pa at 25°C):
3.50x10⁻⁷ (calculated-B.P and ΔHₑₜ, Rordorf 1989)
2.17x10⁻³ (subcooled liquid value, Eitzer & Hites 1988)
Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, log $K_{ow}$:
6.92 (slow stirring-GC/MSD, from fly-ash extract, Sijm et al. 1989a; quoted, Loonen et al. 1991)
7.82 (calculated-QSAR, Fiedler & Schramm 1990)
7.60 (calculated, Broman et al. 1991)

Bioconcentration Factor, log BCF:
3.70 (guppy, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990)

Sorption Partition Coefficient, log $K_{oc}$:
5.59 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
7.40 (calculated, Broman et al. 1991)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination half-life of 108 days in the liver of female rats (Van den Berg et al. 1989); 61, 69 days in rainbow trout at the 0.82 ng/g exposure concentration from 0-140 days data, at 9.0 ng/g exposure concentration from 0-180 days data (Muir et al. 1990); 65 days in whole body rainbow trout with 31 days dietary exposure (Muir et al. 1990); elimination half-life of 48.5 days for lactating cows (Olling et al. 1991); photolytic half-lives in the extract from fly ash in tetradecane solution, calculated to be 3.5 hours for native congener and 3.1 hours for ^13C labelled congener (Tysklind & Rappe 1991).

Environmental Fate Rate Constants or Half-Lives:
Volatilization:
Photolysis: photolytic degradation half-lives of PCDD in extract of fly ash in tetradecane solution, 3.5 hours for native congener and 3.1 hours for ^13C-labelled congener (Tysklind & Rappe 1991).
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_2$: 0.0027 day$^{-1}$ (carp, calculated from data reported by Kuehl et al. 1987, Sijm et al. 1990)

$k_1$: 400 mL gram$^{-1}$ day$^{-1}$ (guppy, Oppenhuizen et al. 1986; quoted, Oppenhuizen & Sijm 1990; Sijm et al. 1990)

$k_2$: 0.079 day$^{-1}$ (guppy, Oppenhuizen et al. 1986; quoted, Oppenhuizen & Sijm 1990; Sijm et al. 1990)

$k_2$: 0.0064 day$^{-1}$ (liver of female rat, Van den Berg et al. 1989)

$k_2$: 10.1x10$^{-3}$ day$^{-1}$ (rainbow trout, 0-140 days exposure at 0.82 ng/g PCDF concn., Muir et al. 1990; quoted, Sijm et al. 1990)

$k_2$: 8.10x10$^{-3}$ day$^{-1}$ (rainbow trout, 0-180 days exposure at 0.82 ng/g PCDF concn., Muir et al. 1990)

$k_2$: 12.6x10$^{-3}$ day$^{-1}$ (rainbow trout, 0-140 days exposure at 9.01 ng/g PCDF concn., Muir et al. 1990;)

$k_2$: 11.4x10$^{-3}$ day$^{-1}$ (rainbow trout, 0-180 days exposure at 9.01 ng/g PCDF concn., Muir et al. 1990)
Common Name: 1,2,3,4,7,8-Hexachlorodibenzofuran
Synonym: 1,2,3,4,7,8-HCDF
Chemical Name: 1,2,3,4,7,8-Hexachlorodibenzofuran
CAS Registry No: 70658-26-9
Molecular Formula: C_{11}H_{2}Cl_{2}OC_{6}Cl_{4}
Molecular Weight: 374.87

Melt Point (°C):
225.5-226.5 (Kuroki et al. 1984)
225.5, 226.5 (quoted, Rordorf 1989)

Boiling Point (°C):
487.7 (calculated, Rordorf 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
310 (LeBas method)

Molecular Volume (Å³):

Total Surface Area, TSA (Å²):
274.71 (van der Waals surface area, Dunn II et al. 1988)

Heat of Fusion, ΔH₂⁰, kcal/mol:
75.76 (Rordorf 1989)

Entropy of Fusion, ΔS₂⁰, cal/mol K (e.u.):
22.94 (Rordorf 1989)

Fugacity Ratio at 25 °C (assuming ΔS = 13.5 e.u.):
0.0103 (at M.P. = 226°C)

Water Solubility (g/m³ or mg/L at 25°C):
8.25x10⁻⁶ (22.7°C, gen. col.-GC/MS, Friessen et al. 1990)

Vapor Pressure (Pa at 25°C):
3.20x10⁻⁸ (calculated, Rordorf 1989)
8.093x10⁻⁶ (subcooled liquid value, GC-RT, Eitzer & Hites 1985)
8.90x10⁻⁶ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
Henry’s Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log $K_{ow}$:
7.70 (calculated, Broman et al. 1991)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{oc}$:
7.40 (calculated, Broman et al. 1991)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: about 336 days in carp (Kuehl et al. 1987); elimination half-life of 48.5 days from lactating cows (Olling et al. 1991).

Environmental Fate Rate Constants or Half-Lives:
Volatilization:
Photolysis: photolytic half-life for the PCDD in extract of fly ash in tetradecane solution, 5.5 hours for native congener (Tysklind & Rappe 1991).

Hydrolysis:
Oxidation: oxidative degradation rate constant of water dissolved PDCF by ozone is $7.28 \times 10^4$ liter gram⁻¹ minute⁻¹ under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987).

Biodegradation:
Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
Common Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran
Synonym: 1,2,3,4,6,7,8-HCDF
Chemical Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran
CAS Registry No: 67462-39-4
Molecular Formula: C₉H₉Cl₉O₅Cl₄
Molecular Weight: 409.31

Melting Point (°C):
236-237 (Kuroki et al. 1984)
236.237 (quoted, Rordorf 1989)

Boiling Point (°C):
507.2 (calculated, Rordorf 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
330.9 (LeBas method)

Molecular Volume (Å³):
Total Surface Area, TSA (Å²):
289.57 (van der Waals surface area, Dunn III et al. 1988)

Heat of Fusion, ΔHₘₒ, kcal/mol:
75.76 (Rordorf 1989)

Entropy of Fusion, ΔSᵣₒ, cal/mol K (e.u.):
25.33 (Rordorf 1989)

Fugacity Ratio at 25°C (assuming ΔS = 13.5 e.u.):
0.00819

Water Solubility (g/m³ or mg/L at 25°C):
1.35x10⁻⁶ (22.7°C, gen. col.-GC/MS, Friessen et al. 1990)
1.08x10⁻⁶ (calculated-QSAR, Fiedler & Schramm 1990)

Vapor Pressure (Pa at 25°C):
4.70x10⁻⁸ (calculated, Rordorf 1989)
2.24x10⁻⁶ (subcooled liquid value, GC-RT, Eitzer & Hites 1988)
1.93x10⁻⁶ (subcooled liquid, Eitzer & Hites 1989)
5.10x10^8 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

Henry’s Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, log K_{ow}:
- 7.92 (slow stirring-GC/MSD, from fly-ash extract, Sijm et al. 1989a)
- 9.25 (calculated-QSAR, Friedler & Schramm 1990)
- 7.90 (quoted, Loonen et al. 1991)
- 8.10 (calculated, Broman et al. 1991)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:
- 6.37 (organic carbon, calculated-QSAR, Friedler & Schramm 1990)
- 6.00 (organic carbon, calculated, Broman et al. 1991)
- 7.90 (calculated, Broman et al. 1991)

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
  - Biota: depuration half-life, > 336 days for carp in Lake Superior water (Keuhl et al. 1987); elimination half-life from lactating cows, 33.9 days (Olling et al. 1991).

Environmental Fate Rate Constants or Half-Lives:
- Volatilization:
- Photolysis: photolytic degradation half-lives with extract of fly ash and in tetradecane solution, 9.8 hours for native congener and 3.7 hours for ^13C-labelled congener (Tysklind & Rappe 1991).
- Hydrolysis:
Oxidation: oxidative degradation rate constant of water dissolved PCDF by ozone is $1.08 \times 10^5$ liter gram$^{-1}$ minute$^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987).

Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran
Synonym: 1,2,3,4,7,8,9-HCDF
Chemical Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran
CAS Registry No: 55673-89-7
Molecular Formula: C_9H_Cl_3OC_6Cl_4
Molecular Weight: 409.31

Melting Point (°C):
221-223 (Kuroki et al. 1984)
221, 223 (quoted, Rordorf 1989)
Boiling Point (°C):
507.2 (calculated, Rordorf 1989)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
330.9 (LeBas method)
Molecular Volume (Å³):
Total Surface Area, TSA (Å²):
285.99 (van der Waals surface area, Dunn III et al. 1988)
Heat of Fusion, kcal/mol:
78.87 (Rordorf 1989)
Entropy of Fusion, cal/mol K (e.u.):
26.05 (Rordorf 1989)
Fugacity Ratio at 25 °C (assuming ΔS = 13.5 e.u.), F:

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C):
6.200×10⁻⁹ (calculated, Rordorf 1989)
1.305×10⁻⁶ (subcooled liquid value, GC-RT, Eitzer & Hites 1988)
1.011×10⁻⁶ (subcooled liquid, Eitzer & Hites 1989)

Henry’s Law Constant (Pa m³/mol):
Common Name: Octachlorodibenzo-furan
Synonym: OCDF
Chemical Name: octachlorodibenzo-furan
CAS Registry No: 39001-02-0
Molecular Formula: C₆Cl₄OC₆Cl₄
Molecular Weight: 443.76

Melting Point (°C):
330 (Doucette 1985)
258-260 (quoted, Rordorf 1986, 1989)

Boiling Point (°C):
510 (calculated, Rordorf 1986)
537 (calculated, Rordorf 1989)

Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
351.8 (LeBas method)

Molar Volume (Å³):

Total Surface Area, TSA (Å²):
298.0 (Doucette 1985, Doucette & Andren 1987)
300.44 (van der Waals surface area, Dunn III et al. 1986)

Heat of Fusion, ΔHₘₙ, kcal/mol:
77.22 (Rordorf 1989)

Entropy of Fusion, ΔSₘₙ, cal/mol K (e.u.):
25.813 (Rordorf 1986, 1989)

Fugacity Ratio at 25 °C (assuming ΔSₘₙ = 13.5 e.u.):
0.00496

Water Solubility (g/m³ or mg/L at 25°C):
1.16x10⁻⁶ (gen. col.-GC, Doucette & Andren 1988a, quoted, Friesen et al. 1990b)
1.54x10⁻⁶ (calculated-QSAR, Fiedler & Schramm 1990)
4.00x10⁻⁸ (quoted, Gobas & Schrap 1990)
Vapor Pressure (Pa at 25°C):
1.90x10^{-7} (quoted, Van den Berg et al. 1985)
5.00x10^{-10} (gas saturation, Rordorf 1989)
2.60x10^{-7} (subcooled liquid, GC/MS, Eitzer & Hites 1989)
5.00x10^{-10} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

Henry's Law Constant (Pa m^3/mol):
0.10 (estimated, Clark & Mackay 1991)

Octanol/Water Partition Coefficient, log K_{ow}:
13.06, 13.22, 13.78; 12.54, 13.37, 13.93 (HPLC-RT, linear regressions; quadratic regressions, Sarna et al. 1984)
8.78 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986; quoted, Geyer et al. 1987)
7.97 (gen. col.-GC/ECD, Doucette & Andren 1987, 1988; quoted, Geyer et al. 1987; Sijm et al. 1989a)
9.96, 6.94 (calculated-f const., TSA, K_{ow}, Doucette & Andren 1987)
9.96 (calculated-QSAR, Fiedler & Schramm 1990)
8.20 (quoted, Gobas & Schrap 1990)
7.60 (calculated, Broman et al. 1991)
7.97 (quoted, Clark & Mackay 1991)

Bioconcentration Factor, log BCF:
1.613, 0.70 (human fat, calculated-different K_{ows}, wet weight basis, Geyer et al. 1987)
1.71, 0.778 (human fat, calculated-different K_{ows}, lipid basis, Geyer et al. 1987)
2.77, 3.89 (guppy, wet weight based, lipid weight based, Gobas & Schrap 1990)

Sorption Partition Coefficient, log K_{oc}:
6.75 (calculated-QSAR, Fiedler & Schramm 1990)
6.00 (organic carbon, calculated, Broman et al. 1991)
7.40 (calculated, Broman et al. 1991)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: mean biological half-life in rainbow trout, about 7 days (Niimi 1986); 7 to 12 days in rainbow trout (Niimi & Oliver 1986; quoted, Muir et al. 1990; Clark & Mackay 1991).

Environmental Fate Rate Constants or Half-Lives:
Volatilization:
Photolysis: photolytic half-life from extract of fly ash in tetradecane solution, 2.1 hours for native congener (Tysklind & Rappe 1991).

Hydrolysis:
Oxidation: oxidative degradation rate for water dissolved OCDF by ozone is 1.05 x 10^4 liter gram^-1 minute^-1 under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987).

Biodegradation:
Biotransformation: metabolism half-time 10^7 hours (guppy, Clark & Mackay 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
\[ k_1 = 0.012 \text{ day}^{-1} \] (rainbow trout, Nimii & Oliver 1986; quoted, Opperhuizen & Sijm 1990)
\[ k_1 = 824 \text{ day}^{-1} \] (guppy, Gobas & Schrap 1990)
\[ k_2 = 1.4 \text{ day}^{-1} \] (guppy, Gobas & Schrap 1990)