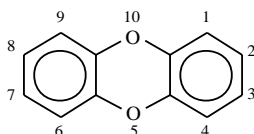


### 3. CHEMICAL AND PHYSICAL INFORMATION

CDDs are a class of related chlorinated hydrocarbons which are structurally similar. The basic structure is a dibenzo-*p*-dioxin (DD) molecule, which is comprised of 2 benzene rings joined at their *para* carbons by 2 oxygen atoms. There are 8 homologues of CDDs, monochlorinated through octachlorinated. The class of CDDs contains 75 congeners, consisting of 2 monochlorodibenzo-*p*-dioxins (MCDDs), 10 dichlorodibenzo-*p*-dioxins (DCDDs), 14 trichlorodibenzo-*p*-dioxins (TrCDDs), 22 tetrachlorodibenzo-*p*-dioxins (TCDDs), 14 pentachlorodibenzo-*p*-dioxins (PeCDD), 10 hexachlorodibenzo-*p*-dioxins (HxCDDs), 2 heptachlorodibenzo-*p*-dioxins (HpCDDs), and a single octachlorodibenzo-*p*-dioxin (OCDD) (Ryan et al. 1991). The general structure of the dibenzo-*p*-dioxins is shown below. The numbers indicate the positions for chlorine substitutions, excluding, of course, positions 5 and 10.



Not all congeners have been studied for their chemical and physical properties, but basic properties are known for the CDDs as a chemical family and for the homologous groups. Chlorinated dioxins exist as colorless solids or crystals in the pure state. They have a low solubility in water and a low volatility. Chlorinated dioxins have an affinity for particulates and readily partition to particles in air, water, and soil. The more toxic compounds appear to be the 2,3,7,8-substituted tetra-, penta-, and hexachloro compounds (i.e., 2,3,7,8-TCDD, 1,2,3,7,8-PeCDD, 1,2,3,4,7,8-HxCDD, 1,2,3,6,7,8-HxCDD, and 1,2,3,7,8,9-HxCDD). These are also the congeners, along with OCDD, that have the greatest tendency to bioaccumulate. One of the most toxic congeners in mammals is believed to be 2,3,7,8-TCDD; this compound has also been the most studied of the TCDD congeners.

#### 3.1 CHEMICAL IDENTITY

Information regarding the chemical identities of CDDs is presented in Table 3-1.

#### 3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of CDDs is presented in Table 3-2.













Table 3-2. Physical and Chemical Properties of CDDs<sup>a</sup> (continued)

Characteristic	Tetrachlorodibenzo-p-dioxins <sup>n</sup>	Pentachlorodibenzo-p-dioxins	Hexachlorodibenzo-p-dioxins
Molecular weight	322	356.4	390.9
Color	White or colorless <sup>b,c</sup> (2,3,7,8-); colorless needles (2,3,7,8-) <sup>k</sup> ; colorless (1,2,3,4-, 1,3,6,8-) <sup>b</sup>	Colorless (1,2,3,4,7-) <sup>b</sup>	Colorless (1,2,3,4,7,8-, 1,2,4,6,7,9-) <sup>b</sup>
Physical state	Crystalline solid <sup>c</sup> (2,3,7,8-)	Solid (1,2,3,4,7-) <sup>b</sup>	Solid (1,2,3,4,7,8-, 1,2,4,6,7,9-) <sup>b</sup>
Melting point	190 °C (1,2,3,4-); 175 °C (1,2,3,7-) <sup>d</sup> ; 219-219.5 °C (1,3,6,8-); 193.5-195 °C (1,3,7,8-); 305-306 °C (2,3,7,8-) <sup>b</sup>	195-196 °C (1,2,3,4,7-); 240-241 °C (1,2,3,7,8-); 205-206 °C (1,2,4,7,8-) <sup>b</sup>	273 °C (1,2,3,4,7,8-) <sup>d</sup> ; 275 °C (1,2,3,4,7,8-) <sup>b</sup> ; 285-286 °C (1,2,3,6,7,8-); 243-244 °C (1,2,3,7,8,9-); 238-240 °C (1,2,4,6,7,9-) <sup>b</sup>
Boiling point	446.5 °C <sup>f</sup> (2,3,7,8-)	No data	No data
Density: at 25 °C	1.827 g/mL <sup>g</sup> (2,3,7,8-)	No data	No data
Odor	No data	No data	No data
Odor threshold: Water	No data	No data	No data
Air	No data	No data	No data
Solubility: Water at 25 °C	4.7x10 <sup>-4</sup> -6.3x10 <sup>-4</sup> mg/L (1,2,3,4-) <sup>d,i</sup> 4.2x10 <sup>-4</sup> mg/L (20°C) (1,2,3,7-); 3.2x10 <sup>-4</sup> mg/L (20°C) (1,3,6,8-); 1.9x10 <sup>-5</sup> mg/L (2,3,7,8) <sup>f</sup> 7.9x10 <sup>-6</sup> -3.2x10 <sup>-4</sup> mg/L (2,3,7,8-) <sup>d</sup>	1.18x10 <sup>-4</sup> mg/L (20°C) (1,2,3,4,7-) <sup>d</sup>	4.42x10 <sup>-6</sup> mg/L (20°C) (1,2,3,4,7,8-) <sup>d</sup>
Organic solvent(s) <sup>p</sup>	<i>o</i> -dichlorobenzene, chloro- benzene, benzene, chloroform, <i>n</i> - octanol <sup>b</sup>	No data	No data
Partition coefficients: Log K <sub>ow</sub>	7.02-8.7 (1,2,3,7-) <sup>i,e</sup> ; 7.02 (2,3,7,8-) <sup>d</sup> ; 7.39-7.58 (2,3,7,8-); 6.8 (2,3,7,8-TCDD) <sup>m</sup> ; 6.6 (1,2,3,4- TCDD) <sup>m</sup>	8.64-9.48 (1,2,3,4,7-) <sup>d</sup>	9.19-10.4 (1,2,3,4,7,8-) <sup>f</sup>
Log K <sub>oc</sub>	No data	No data	No data



Table 3-2. Physical and Chemical Properties of CDDs<sup>a</sup> (continued)

Characteristic	Tetrachlorodibenzo-p-dioxins <sup>n</sup>	Pentachlorodibenzo-p-dioxins	Hexachlorodibenzo-p-dioxins
Vapor pressure at 25 °C	7.5x10 <sup>-9</sup> mm Hg (1,2,3,7-) <sup>d</sup> ; 4.8x10 <sup>-8</sup> mm Hg (1,2,3,4-) <sup>e</sup> ; 1.5x10 <sup>-9</sup> -3.4x10 <sup>-5</sup> mm Hg (2,3,7,8-) <sup>e</sup> ; 5.3x10 <sup>-9</sup> -4.0x10 <sup>-3</sup> mm Hg (1,3,6,8-) <sup>d</sup> ; 7.4x10 <sup>-10</sup> mm Hg (2,3,7,8-) <sup>k</sup>	6.6x10 <sup>-10</sup> mm Hg (1,2,3,4,7-) <sup>d</sup>	3.8x10 <sup>-11</sup> mm Hg (1,2,3,4,7,8-) <sup>d</sup>
Henry's law constant at 25 °C	16.1x10 <sup>-6</sup> -101.7x10 <sup>-6</sup> atm·m <sup>3</sup> /mol (2,3,7,8-); 7.01x10 <sup>-6</sup> -101.7x10 <sup>-6</sup> atm·m <sup>3</sup> /mol <sup>d</sup>	2.6x10 <sup>-6</sup> atm·m <sup>3</sup> /mol (1,2,3,4,7-) <sup>d</sup>	44.6x10 <sup>-6</sup> atm·m <sup>3</sup> /mol (1,2,3,4,7,8-) <sup>d</sup>
Degradation	photodegradation half-life on grass (2,3,7,8-)=44 h(k <sub>2</sub> = 0.0156 h <sup>-1</sup> ) <sup>m,o</sup> ; atmospheric lifetime using gas-phase reaction with OH radical = 0.8 to 2 days <sup>q</sup>	atmospheric lifetime using gas- phase reaction with OH radical = 1.1 to 2.4 days <sup>q</sup>	atmospheric lifetime using gas- phase reaction with OH radical = 1.5 to 3.4 days <sup>q</sup>
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors in air at 25 °C, 760 mm Hg	1 mg/m <sup>3</sup> = 0.0759 ppm 1 ppm = 13.17 mg/m <sup>3</sup>	1 mg/m <sup>3</sup> = 0.0686 ppm 1 ppm = 14.58 mg/m <sup>3</sup>	1 mg/m <sup>3</sup> = 0.0625 ppm 1 ppm = 15.99 mg/m <sup>3</sup>
Explosive limits	No data	No data	No data

Table 3-2. Physical and Chemical Properties of CDDs<sup>a</sup> (continued)

Characteristic	Heptachlorodibenzo-p-dioxins	Octachlorodibenzo-p-dioxin
Molecular weight	425.3	459.8
Color	No data	No data
Physical state	No data	No data
Melting point	265 °C (1,2,3,4,6,7,8-) <sup>d</sup>	332 °C <sup>d</sup> ; 330 °C <sup>k</sup>
Boiling point	507.2 °C <sup>e</sup>	510 °C <sup>a</sup> ; 485 °C <sup>m</sup>
Density: at 25 °C	No data	No data
Odor	No data	No data
Odor threshold: Water Air	No data No data	No data No data
Solubility: Water at 25 °C	2.4x10 <sup>-6</sup> mg/L at 20°C (1,2,3,4,6,7,8-) <sup>d</sup> ; 1.9x10 <sup>-3</sup> mg/L at 20°C (b,e)(1,4) <sup>k</sup>	7.4x10 <sup>-8</sup> mg/L <sup>d</sup> ; 0.4±0.1x10 <sup>-9</sup> g/L at 20 °C <sup>k</sup> ; 2.27x10 <sup>-9</sup> mg/L <sup>m</sup>
Organic solvent(s) <sup>p</sup>	No data	Acetic acid, anisole, chloroform, <u>o</u> -dichlorobenzene, dioxane, diphenyl oxide, pyridine, xylene <sup>b</sup>
Partition coefficients: Log K <sub>ow</sub>	9.69–11.38 (1,2,3,4,6,7,8-) <sup>f</sup>	10.07–12.26 <sup>f</sup> ; 8.78-13.37 <sup>k</sup>
Log K <sub>oc</sub>	No data	No data
Vapor pressure at 25 °C	5.6x10 <sup>-12</sup> mm Hg; (1,2,3,4,6,7,8-) <sup>e</sup> ; 7.4x10 <sup>-8</sup> mm Hg (b,e)(1,4) <sup>k</sup>	8.25x10 <sup>-13</sup> mm Hg <sup>e</sup> ; 1.68x10 <sup>-12</sup> <sup>m</sup>
Henry's law constant at 25 °C	1.31x10 <sup>-6</sup> atm·m <sup>3</sup> /mol (1,2,3,4,6,7,8-) <sup>d</sup> ; 2.18x10 <sup>-5</sup> atm·m <sup>3</sup> /mol <sup>k</sup>	6.74x10 <sup>-6</sup> atm·m <sup>3</sup> /mol <sup>d,k</sup>

Table 3-2. Physical and Chemical Properties of CDDs<sup>a</sup> (continued)

Characteristic	Heptachlorodibenzo-p-dioxins	Octachlorodibenzo-p-dioxin
Degradation	Atmospheric lifetime using gas-phase reaction with OH radical = 4.4 days <sup>q</sup>	Atmospheric lifetime using gas-phase reaction with OH radical = 9.6 days <sup>q</sup>
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	No data	No data
Conversion factors in air at 25 °C, 760 mm Hg	1 mg/m <sup>3</sup> = 0.0575 ppm 1 ppm = 17.39 mg/m <sup>3</sup>	1 mg/m <sup>3</sup> = 0.0532 ppm 1 ppm = 18.81 mg/m <sup>3</sup>
Explosive limits	No data	No data

<sup>a</sup> In some cases, information regarding chemical and physical properties was not available for all isomers of a homologous class

<sup>b</sup> IARC 1977

<sup>c</sup> Sax and Lewis 1987

<sup>d</sup> Shiu et al. 1988

<sup>e</sup> Rordorf 1989

<sup>f</sup> Webster et al. 1985

<sup>g</sup> Schroy et al. 1985

<sup>h</sup> Solubility is given for 25 °C unless noted otherwise in text.

<sup>i</sup> Doucette and Andren 1988

<sup>j</sup> Des Rosiers 1986

<sup>k</sup> HSDB 1995

<sup>l</sup> ASTER 1995

<sup>m</sup> McCrady and Maggard 1993

<sup>n</sup> Physical & chemical properties of 2,3,7,8-TCDD are shown in bold

<sup>o</sup>  $k_2$  = elimination rate constants

<sup>p</sup> In most cases no specific solubilities were found. However, solvation in organic solvents such as toluene, hexane and methylene chloride is possible given that these solvents are used in extraction and analysis methods (see Chapter 6).

<sup>q</sup> Atkinson 1991

<sup>r</sup> Marple et al. 1986b

