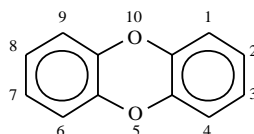


### 3. CHEMICAL AND PHYSICAL INFORMATION

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 3-1. Chemical Identity of CDDs<sup>a</sup>

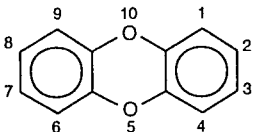
| Characteristic                                       | Monochlorodibenzo-p-dioxins   | Dichlorodibenzo-p-dioxins  |
|--|---|--|
| Chemical Name  | 1-Chlorodibenzo-p-dioxin (CAS #39227-53-7);<br>2-Chlorodibenzo-p-dioxin (CAS #39227-54-8) <sup>b</sup>  | 2,7-Dichlorobenzo-p-dioxin(CAS #33857-26-0) <sup>e</sup>   |
| Synonym(s) <sup>j</sup>                              | 1-Chlorodibenzo-p-dioxin; 1-Chlorodibenzo-p-dioxin;<br>1-Chlorodibenzo[b,e](1,4)dioxin <sup>c</sup> ; 2-Chlorodi-<br>benzo(b,e)(1,4)dioxin <sup>b</sup> | 1,3- or 1,6- or 2,3- or 2,7- or 2,8-Dichlorodibenzo-p-<br>dioxin; 1,3- or 1,6- or 2,3- or 2,7- or 2,8-Dichlorodiben-<br>zo[b,e](1,4)dioxin; 1,3- or 1,6- or 2,3- or 2,7- or 2,8-<br>Dichlorodibenzodioxin <sup>b</sup> |
| Total number of possible isomers                     | 2   | 10   |
| Registered trade name(s)                             | No data   | No data  |
| Chemical formula                                     | C <sub>12</sub> H <sub>7</sub> ClO <sub>2</sub> <sup>c</sup>  | C <sub>12</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub> <sup>b</sup>   |
| Chemical structure <sup>b,i</sup>                    |    | See footnote "f"   |
| Identification numbers: <sup>h</sup><br>CAS registry | 39227-53-7 (1-) <sup>c</sup><br>39227-54-8 (2-) <sup>b</sup>  | 50585-39-2 (1,3-);<br>38178-38-0 (1,6-);<br>29446-15-9 (2,3-) <sup>c</sup> ;<br>33857-26-0 (2,7-) <sup>e</sup> ;<br>38964-22-6 (2,8-) <sup>c</sup>   |
| NIOSH RTECS  | HP3095300 (1-);<br>HP3095500 (2-) <sup>c</sup>  | HP3095700 (1,3-);<br>HP3095800 (1,6-);<br>HP3096000 (2,3-) <sup>c</sup> ;<br>HP3100000 (2,7-) <sup>e</sup> ;<br>HP3150000 (2,8-) <sup>c</sup>  |
| EPA hazardous waste                                  | No data   | No data  |
| OHM/TADS   | No data   | No data  |
| DOT/UN/NA/IMCO shipping                              | No data   | No data  |
| HSDB   | No data   | 4124 (2,7-) <sup>e</sup>   |
| NCI  | No data   | CO3667 (2,7-) <sup>e</sup>   |

Table 3-1. Chemical Identity of CDDs<sup>a</sup> (continued)

| Characteristic                                       | Trichlorodibenzo- <i>p</i> -dioxins  | Tetrachlorodibenzo- <i>p</i> -dioxins <sup>g</sup>   |
|--|--|--|
| Chemical name  | 1,2,4-Trichlorodibenzo- <i>p</i> -dioxin (CAS # 39227-58-2);<br>2,3,7-Trichlorodibenzo- <i>p</i> -dioxin (CAS # 33857-28-2) <sup>b</sup>                     | 2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin (CAS # 1746-01-6) <sup>g</sup>  |
| Synonym(s) <sup>l</sup>                              | 1,2,4- or 2,3,7-Trichlorodibenzo- <i>para</i> -dioxin; 1,2,4- or 2,3,7-Trichlorodibenzo[b,e](1,4)dioxin; 1,2,4- or 2,3,7-Trichlorodibenzodioxin <sup>b</sup> | 1,2,3,4- or 1,2,3,8- or 1,3,6,8- or 1,3,7,8- or 1,2,7,8- or 2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin <sup>d</sup> ; 1,2,3,4- or 1,2,3,8- or 1,2,7,8- or 1,3,6,8- or 1,3,7,8- or 2,3,7,8-Tetrachlorodibenzodioxin; 1,2,3,4- or 1,2,3,8- or 1,3,6,8- or 1,3,7,8- or 1,2,7,8- or 2,3,7,8-Tetrachlorodibenzo[b,e](1,4)dioxin; 1,2,7,8- or 2,3,7,8-Tetrachlorodibenzo-1,4-dioxin; 2,3,6,7-Tetrachloro-dibenzodioxin; 1,2,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin; Dioxin; TCDBD; TCDD <sup>b</sup> |
| Total number of possible isomers                     | 14   | 22   |
| Registered trade name(s)                             | No data  | No data  |
| Chemical formula                                     | C <sub>12</sub> H <sub>5</sub> Cl <sub>3</sub> O <sub>2</sub> <sup>e,i</sup>   | C <sub>12</sub> H <sub>4</sub> Cl <sub>4</sub> O <sub>2</sub> <sup>b</sup>   |
| Chemical structure <sup>b,i</sup>                    | See footnote "f"   | See footnote "f"   |
| Identification numbers: <sup>h</sup><br>CAS registry | 39227-58-2 (1,2,4-);<br>33857-28-2 (2,3,7-) <sup>c</sup>   | 30746-58-8 (1,2,3,4-);<br>53555-02-5 (1,2,3,8-);<br>34816-53-0 (1,2,7,8-);<br>33423-92-6 (1,3,6,8-);<br>50585-46-1 (1,3,7,8-) <sup>c</sup><br><b>1746-01-6 (2,3,7,8-)<sup>e</sup></b>  |
| NIOSH RTECS  | HP3530000 (1,2,4-);<br>HP3630000 (2,3,7-) <sup>c</sup>   | HP3493000 (1,2,3,4-);<br>HP3494000 (1,2,3,8-);<br>HP3494500 (1,2,7,8-);<br>HP3495000 (1,3,6,8-);<br>HP3495500 (1,3,7,8-) <sup>c</sup> ;<br><b>HP3500000 (2,3,7,8-)<sup>e</sup></b>   |
| EPA hazardous waste                                  | No data  | No data  |
| OHM/TADS   | No data  | No data  |
| DOT/UN/NA/IMCO shipping                              | No data  | No data  |
| HSDB   | No data  | 4151 (2,3,7,8-) <sup>e</sup>   |
| NCI  | No data  | C03714 (2,3,7,8-) <sup>e</sup>   |

Table 3-1. Chemical Identity of CDDs<sup>a</sup> (continued)

| Characteristics                                      | Pentachlorodibenzo-p-dioxins   | Hexachlorodibenzo-p-dioxins  |
|--|--|--|
| Chemical name  | 1,2,3,7,8-Pentachlorodibenzo-p-dioxin (CAS #40321-76-4) <sup>c</sup>   | 1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin (CAS #57653-85-7); 1,2,3,7,8,9- Hexachlorodibenzo-p-dioxin (CAS #19408-74-3); Hexachlorodibenzo-p-dioxin (CAS #34465-46-8) <sup>e</sup>   |
| Synonym(s) <sup>f</sup>                              | 1,2,3,4,7- or 1,2,3,7,8- or 1,2,4,7,8-Pentachlorodibenzo-para-dioxin; 1,2,3,4,7- or 1,2,3,7,8- or 1,2,4,7,8-Pentachlorodibenzodioxin; 1,2,3,4,7- or 1,2,3,7,8- or 1,2,4,7,8-Pentachlorodibenzo[b,e] (1,4)dioxin <sup>b</sup> | 1,2,3,4,7,8- or 1,2,3,6,7,8- or 1,2,3,6,7,9- or 1,2,3,7,8,9- or 1,2,4,6,7,9-Hexachlorodi-benzo-para-dioxin; 1,2,3,4,7,8- or 1,2,3,6,7,8- or 1,2,3,6,7,9- or 1,2,3,7,8,9- or 1,2,4,6,7,9-Hexachlorodibenzodioxin <sup>b</sup> ; Hexachlorodibenzo(b,e) (1,4)dioxin <sup>i</sup> ; Hexachlorodibenzo-4-dioxin <sup>e</sup> |
| Total number of possible isomers                     | 14   | 10   |
| Registered trade name(s)                             | No data  | No data  |
| Chemical formula                                     | C <sub>12</sub> H <sub>3</sub> Cl <sub>5</sub> O <sub>2</sub> <sup>c</sup>   | C <sub>12</sub> H <sub>2</sub> Cl <sub>6</sub> O <sub>2</sub> <sup>b</sup>   |
| Chemical structure <sup>b,f</sup>                    | See footnote "f"   | See footnote "f"   |
| Identification numbers: <sup>h</sup><br>CAS registry | 39227-61-7 (1,2,3,4,7-);<br>40321-76-4 (1,2,3,7,8-);<br>58802-08-7 (1,2,4,7,8-) <sup>c</sup>   | 57653-85-7 (1,2,3,6,7,8-) <sup>e</sup> ;<br>64461-98-9 (1,2,3,6,7,9-) <sup>c</sup> ;<br>19408-74-3 (1,2,3,7,8,9-) <sup>e</sup> ;<br>39227-62-8 (1,2,4,6,7,9-) <sup>e</sup> ;<br>34465-46-8 <sup>e</sup>  |
| NIOSH RTECS  | HP3370000 (1,2,3,4,7-);<br>HP3395000 (1,2,3,7,8-);<br>HP3420000 (1,2,4,7,8-) <sup>c</sup>  | HP3280000 (1,2,3,4,7,8-);<br>HP3280100 (1,2,3,6,7,8-);<br>HP3290000 (1,2,3,6,7,9-);<br>HP3310000 (1,2,3,7,8,9-);<br>HP3313000 (1,2,4,6,7,9-) <sup>c</sup>  |
| EPA hazardous waste                                  | No data  | No data  |
| OHM/TADS   | No data  | No data  |
| DOT/UN/NA/IMCO shipping                              | No data  | No data  |
| HSDB   | No data  | 4154 (1,2,3,6,7,8-) <sup>e</sup> ; 6867 <sup>e</sup> ; 6866 (1,2,3,7,8,9-) <sup>e</sup>  |
| NCI  | No data  | CO3703 (1,2,3,6,7,8-) <sup>e</sup>   |

Table 3-1. Chemical Identity of CDDs<sup>a</sup> (continued)

| Characteristic                       | Heptachlorodibenzo-p-dioxins   | Octachlorodibenzo-p-dioxin   |
|--------------------------------------|--|--|
| Chemical name                        | Heptachlorodibenzo-p-dioxin (CAS #37871-00-4) <sup>a</sup>   | Octachlorodibenzo-p-dioxin <sup>a</sup>  |
| Synonym(s)                           | 1,2,3,4,6,7,8- or 1,2,3,4,6,7,9-Heptachlorodibenzo-p-dioxin; 1,2,3,4,6,7,8- or 1,2,3,4,6,7,9-Heptachlorodibenzo[b,e](1,4) dioxin; 1,2,3,4,6,7,8- or 1,2,3,4,6,7,9-Heptachlorodibenzo-dioxin; 1,2,3,4,6,7,8- or 1,2,3,4,6,7,9-Heptachlorodibenzo-para-dioxin <sup>c</sup> ; Heptachlorodibenzo(b,e)(1,4)dioxin <sup>e</sup> | 1,2,3,4,6,7,8,9-Octachlorodibenzo-p-dioxin; OCDD; Octachlorodibenzodioxin; Octachlorodibenzo[b,e](1,4)dioxin; Octachlorodibenzo-p-dioxin; 1,2,3,4,6,7,8,9-Octachlorodibenzodioxin; 1,2,3,4,6,7,8,9-Octachlorodibenzo(b,e)(1,4)dioxin; Octachloro-para-dibenzodioxin <sup>b</sup> |
| Total number of possible isomers     | 2  | 1  |
| Registered trade name(s)             | No data  | No data  |
| Chemical formula                     | C <sub>12</sub> HCl <sub>7</sub> O <sub>2</sub> <sup>c</sup>   | C <sub>12</sub> Cl <sub>8</sub> O <sub>2</sub> <sup>e</sup>  |
| Chemical structure <sup>b,f</sup>    | See footnote "f"   | See footnote "f"   |
| Identification numbers: <sup>h</sup> |  |  |
| CAS registry                         | 35822-46-9 (1,2,3,4,6,7,8-) <sup>l</sup> ; 58200-70-7 (1,2,3,4,6,7,9-) <sup>c</sup> ; 37871-00-4 (b,e)(1,4) <sup>e</sup>   | 3268-87-9 <sup>e</sup>   |
| NIOSH RTECS                          | HP3190000 (1,2,3,4,6,7,8-) <sup>c</sup> ;  | HP3350000 <sup>e</sup>   |
| EPA hazardous waste                  | No data  | No data  |
| OHM/TADS                             | No data  | No data  |
| DOT/UN/NA/IMCO shipping              | No data  | No data  |
| HSDB                                 | 6474 (1,2,3,4,6,7,9-)(b,e)(1,4) <sup>e</sup>   | 6480 <sup>e</sup>  |
| NCI                                  | No data  | CO3678 <sup>e</sup>  |

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

<sup>b</sup> IARC 1977

<sup>c</sup> RTECS 1996

<sup>d</sup> 1,2,7,8- is the same isomer as 2,3,6,7-in tetrachlorodibenzo-p-dioxins

<sup>e</sup> HSDB 1995

<sup>f</sup> The structural formula of unsubstituted dibenzo-para-dioxin and the numbering of the carbon atoms in the ring are given under monochlorodibenzo-p-dioxins. The chlorinated dibenzo-para-dioxins contain chlorine atoms at the positions indicated in their names (IARC 1977).

<sup>g</sup> Chemical identity information for 2,3,7,8-TCDD is shown in bold.

<sup>h</sup> Specific chlorine substitutions are given in parentheses following the identification numbers when multiple identification numbers are given

<sup>i</sup> Aster 1995

<sup>j</sup> Example, alternative nomenclature shown; not all possible isomers are listed but can be extrapolated from the general structure or from the literature (Ryan et al. 1991)

CAS = Chemical Abstracts Services; CDDs = chlorinated dibenzo-p-dioxins; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

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

| Characteristic                                 | Monochlorodibenzo-p-dioxins                            | Dichlorodibenzo-p-dioxins   | Trichlorodibenzo-p-dioxins   |
|--|--|---|--|
| Molecular weight                               | 218.6  | 253.1   | 287.5  |
| Color  | Colorless <sup>b</sup>                                 | Colorless <sup>b,k</sup>  | Colorless (1,2,4-) <sup>b</sup>  |
| Physical state                                 | Crystals (1-); solid (2-) <sup>b</sup>                 | Needles (1,6-); solid (2,3-, 2,8-); crystals (2,7-) <sup>b</sup>  | Solid (1,2,4-) <sup>b</sup>  |
| Melting point                                  | 105.5 °C (1-); 89.0 °C (2-) <sup>d</sup>               | 114-115 °C (1,3-); 184-185 °C (1,6-) <sup>b</sup> ; 164 °C (2,3-); 210 °C (2,7); 151 °C (2,8-) <sup>d</sup> | 129 °C (1,2,4-) <sup>d</sup> ; 128-129 °C (1,2,4-) <sup>b</sup> ; 153-163 °C (2,3,7-) <sup>b</sup> |
| Boiling point                                  | No data  | No data   | 374 °C <sup>l</sup>  |
| Density:<br>at 25 °C                           | No data  | No data   | No data  |
| Odor   | No data  | No data   | No data  |
| Odor threshold:<br>Water                       | No data  | No data   | No data  |
| Air  | No data  | No data   | No data  |
| Solubility:<br>Water at 25 °C <sup>h</sup>     | 0.417 mg/L (1-);<br>0.278-0.318 mg/L (2-) <sup>d</sup> | 0.0149 mg/L (2,3-); 0.00375 mg/L (2,7-); 0.0167 mg/L (2,8-) <sup>d</sup>                                    | 0.00841 mg/L (1,2,4-) <sup>d</sup> ;<br>4.75x10 <sup>-3</sup> mg/L <sup>l</sup>                    |
| Organic solvent(s) <sup>p</sup>                | No data  | No data   | No data  |
| Partition coefficients:<br>Log K <sub>ow</sub> | 4.52-5.45 (1-,2-) <sup>f</sup>                         | 5.86-6.39 (2,7-) <sup>f</sup>   | 6.86-7.45 (1,2,4-) <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                                   | Monochlorodibenzo-p-dioxins  | Dichlorodibenzo-p-dioxins  | Trichlorodibenzo-p-dioxins   |
|--|--|--|--|
| Vapor pressure at 25 °C                          | 9.0x10 <sup>-5</sup> mm Hg (1-);<br>1.3x10 <sup>-4</sup> mm Hg (2-) <sup>e</sup>             | 2.9x10 <sup>-6</sup> mm Hg (2,3-);<br>9.0x10 <sup>-7</sup> mm Hg (2,7-);<br>1.1x10 <sup>-6</sup> mm Hg (2,8-) <sup>e</sup> | 2.7x10 <sup>-7</sup> mm Hg (1,3,7-);<br>7.5x10 <sup>-7</sup> mm Hg (1,2,4-) <sup>e</sup> ;<br>6.46 x 10 <sup>-8</sup> mm Hg <sup>l</sup> |
| Henry's law constant<br>at 25 °C                 | 82.7x10 <sup>-6</sup> to 146.26x10 <sup>-6</sup><br>atm·m <sup>3</sup> /mol <sup>d</sup>     | 21.02x10 <sup>-6</sup> to 80.04x10 <sup>-6</sup><br>atm·m <sup>3</sup> /mol (2,3-, 2,7-, 2,8-) <sup>d</sup>                | 37.9x10 <sup>-6</sup> atm·m <sup>3</sup> /mol (1,2,4-) <sup>d</sup>  |
| Degradation                                      | atmospheric lifetime using gas-<br>phase reaction with OH radical =<br>0.5 days <sup>q</sup> | atmospheric lifetime using gas-<br>phase reaction with OH radical =<br>0.5 to 0.7 days <sup>q</sup>                        | atmospheric lifetime using gas-<br>phase reaction with OH radical =<br>0.7 to 0.9 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<br>at 25 °C, 760 mm Hg | 1 mg/m <sup>3</sup> = 0.112 ppm;<br>1 ppm = 8.94 mg/m <sup>3</sup>                           | 1 mg/m <sup>3</sup> = 0.0966 ppm;<br>1 ppm = 10.35 mg/m <sup>3</sup>   | 1 mg/m <sup>3</sup> = 0.0850 ppm;<br>1 ppm = 11.76 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                  | 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-);<br>175 °C (1,2,3,7-) <sup>d</sup> ;<br>219-219.5 °C (1,3,6,8-);<br>193.5-195 °C (1,3,7,8-);<br>305-306 °C (2,3,7,8-) <sup>b</sup>   | 195-196 °C (1,2,3,4,7-);<br>240-241 °C (1,2,3,7,8-);<br>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:<br>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><br>4.2x10 <sup>-4</sup> mg/L (20 °C) (1,2,3,7-);<br>3.2x10 <sup>-4</sup> mg/L (20 °C) (1,3,6,8-);<br>1.9x10 <sup>-5</sup> mg/L (2,3,7,8) <sup>f</sup><br>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)<br>(1,2,3,4,7-) <sup>d</sup>                              | 4.42x10 <sup>-6</sup> mg/L (20 °C)<br>(1,2,3,4,7,8-) <sup>d</sup>  |
| Organic solvent(s) <sup>p</sup> | o-dichlorobenzene, chloro-<br>benzene, benzene, chloroform, n-<br>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<br>(2,3,7,8-) <sup>d</sup> ; 7.39-7.58 (2,3,7,8-);<br>6.8 (2,3,7,8-TCDD) <sup>m</sup> ; 6.6 (1,2,3,4-<br>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<br>at 25 °C                       | 7.5x10 <sup>-9</sup> mm Hg (1,2,3,7-) <sup>d</sup> ;<br>4.8x10 <sup>-8</sup> mm Hg (1,2,3,4-) <sup>e</sup> ;<br>1.5x10 <sup>-9</sup> -3.4x10 <sup>-5</sup> mm Hg<br>(2,3,7,8-) <sup>e</sup> ; 5.3x10 <sup>-9</sup> -4.0x10 <sup>-3</sup> mm<br>Hg (1,3,6,8-) <sup>d</sup> ; 7.4x10 <sup>-10</sup> mm Hg<br>(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<br>at 25 °C                 | 16.1x10 <sup>-6</sup> -101.7x10 <sup>-6</sup> atm·m <sup>3</sup> /mol<br>(2,3,7,8-); 7.01x10 <sup>-6</sup> -101.7x10 <sup>-6</sup><br>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<br>(1,2,3,4,7,8-) <sup>d</sup>                        |
| Degradation                                      | photodegradation half-life on<br>grass (2,3,7,8-)=44 h(k <sub>2</sub> = 0.0156<br>h <sup>-1</sup> ) <sup>m,o</sup> ; atmospheric lifetime using<br>gas-phase reaction with OH<br>radical = 0.8 to 2 days <sup>q</sup>  | atmospheric lifetime using gas-<br>phase reaction with OH radical =<br>1.1 to 2.4 days <sup>q</sup> | atmospheric lifetime using gas-<br>phase reaction with OH radical =<br>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<br>at 25 °C, 760 mm Hg | 1 mg/m <sup>3</sup> = 0.0759 ppm<br>1 ppm = 13.17 mg/m <sup>3</sup>  | 1 mg/m <sup>3</sup> = 0.0686 ppm<br>1 ppm = 14.58 mg/m <sup>3</sup>                                 | 1 mg/m <sup>3</sup> = 0.0625 ppm<br>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:<br>at 25 °C             | No data   | No data  |
| Odor                             | No data   | No data  |
| Odor threshold:                  |   |  |
| Water                            | No data   | No data  |
| Air                              | 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> ;<br>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> ;<br>2.27x10 <sup>-9</sup> mg/L <sup>m</sup> |
| Organic solvent(s) <sup>p</sup>  | No data   | Acetic acid, anisole, chloroform, <i>o</i> -dichlorobenzene,<br>dioxane, diphenyl oxide, pyridine, xylene <sup>b</sup>                   |
| Partition coefficients:          |   |  |
| Log K <sub>ow</sub>              | 9.69–11.38<br>(1,2,3,4,6,7,8-) <sup>i</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> ;<br>7.4x10 <sup>-8</sup> mm Hg (b,e)(1,4) <sup>k</sup>                          | 8.25x10 <sup>-13</sup> mm Hg <sup>g</sup> ; 1.68x10 <sup>-12</sup> m   |
| Henry's law constant<br>at 25 °C | 1.31x10 <sup>-6</sup> atm·m <sup>3</sup> /mol (1,2,3,4,6,7,8-) <sup>d</sup> ;<br>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<br>1 ppm = 17.39 mg/m <sup>3</sup>                   | 1 mg/m <sup>3</sup> = 0.0532 ppm<br>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

