#### **CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION**

#### 4.1 CHEMICAL IDENTITY

Dibenzofuran is an organic compound that contains two benzene rings fused to a central furan ring. CDFs are a class of organic compounds in which one to eight chlorine atoms are attached to the benzene ring positions of a dibenzofuran structure.

Based on the number of chlorine substituents (one to eight) on the benzene rings, there are eight homologues of CDFs (monochlorinated through octachlorinated). Each homologous group contains one or more isomers. There are 135 possible CDF isomers, including 4 monoCDFs, 16 diCDFs, 28 triCDFs, 38 tetraCDFs, 28 pentaCDFs, 16 hexaCDFs, 4 heptaCDFs, and 1 octaCDF. Each one of these compounds is called a congener. Because of molecular asymmetry, CDFs have 135 congeners, compared to 75 for CDDs.

The synonyms, chemical formulas, chemical structure, and identification numbers of selected CDFs are reported in Table 4-1. CDFs that are known or suspected to be most toxic (2,3,7,8-substituted congeners) and other CDFs, for which health effects data are discussed in Chapter 2, have been selected for inclusion in Table 4-1.

#### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

CDFs have been synthesized in quantities <1 g. The methods needed to separate the isomeric compounds in a congener series make the isolation of an individual congener difficult. Therefore, data pertaining to the simplest physical and chemical properties of the individual congener are not generally available. The extremely low water solubilities and vapor pressures contribute to the difficulty in determining these and related physico-chemical properties (e.g., K<sub>ow</sub> and Henry's law constant) of these compounds. In general, the melting point increases and the vapor pressures and water solubilities of the CDFs decrease as the number of chlorine substituents increases (see Table 4-2). These hydrophobic compounds are generally colorless solids and are soluble in nonpolar organic solvents (Gray et al. 1976). The CDFs are relatively stable towards acid and alkali attack, but they start to decompose at 700°C (van den Berg et al. 1985). The physical and chemical properties of CDFs are given in Table 4-2.

	Table 4-1. Chemic	al Identity of Chlorodi	benzofurans (CDFs)	
Characteristic		Infor	mation	
Chemical name	1,3,7,8-TetraCDF	2,3,6,8-TetraCDF	2,3,7,8-TetraCDF	1,2,3,4,8-PentaCDF
Registered trade name(s)	No data	No data	No data	No data
Chemical formula	C <sub>12</sub> H <sub>4</sub> Cl <sub>4</sub> O	C <sub>12</sub> H <sub>4</sub> Cl <sub>4</sub> O	C <sub>12</sub> H <sub>4</sub> Cl <sub>4</sub> O	C <sub>12</sub> H <sub>3</sub> Cl <sub>5</sub> O
Chemical structure		CI CI CI	CI CI O CI	
CAS Registry Number <sup>a</sup>	57117-35-8	57117-37-0	51207-31-9	67517-48-0
Chemical name	1,2,3,7,8-PentaCDF	2,3,4,7,8-PentaCDF	1,2,3,4,7,8-HexaCDF	1,2,3,6,7,8-HexaCDF
Registered trade name(s)	No data	No data	No data	No data
Chemical formula	C <sub>12</sub> H <sub>3</sub> Cl <sub>5</sub> O	$C_{12}H_3CI_5O$	$C_{12}H_2CI_6O$	$C_{12}H_2CI_6O$
Chemical structure		CI CI CI		
CAS Registry Number <sup>a</sup>	57117-41-6	57117-31-4	70648-26-9	57117-44-9
Chemical name	1,2,3,7,8,9-HexaCDF	1,2,4,6,7,9-HexaCDF	2,3,4,6,7,8-HexaCDF	1,2,3,4,6,7,8-HeptaCDF
Registered trade name(s)	No data	No data	No data	No data
Chemical formula				
Chemical structure	C <sub>12</sub> H <sub>2</sub> Cl <sub>6</sub> O	C <sub>12</sub> H <sub>2</sub> Cl <sub>6</sub> O	C <sub>12</sub> H <sub>2</sub> Cl <sub>6</sub> O	C <sub>12</sub> HCI7O
CAS Registry Number <sup>a</sup>	72918-21-9	75627-02-0	60851-34-5	67562-39-4

### Table 4-1. Chemical Identity of Chlorodibenzofurans (CDFs)

	Table 4-1. Chemi	ical Identity of Chlorod	ibenzofurans (CDFs)	
Characteristic		Info	ormation	
Chemical name	1,2,3,4,6,7,9-HeptaCDF	1,2,3,4,6,8,9-HeptaCDF	1,2,3,4,7,8,9-HeptaCDF	1,2,3,4,6,7,8,9-OctaCDF
Registered trade name(s)	No data	No data	No data	No data
Chemical formula	C <sub>12</sub> HCI <sub>7</sub> O	C <sub>12</sub> HCl <sub>7</sub> O	C <sub>12</sub> HCl <sub>7</sub> O	C <sub>12</sub> Cl <sub>8</sub> O
Chemical structure				
CAS Registry Number <sup>a</sup>	70648-25-8	69698-58-4	55673-89-7	39001-02-0

<sup>a</sup>EPA 1985

CAS = Chemical Abstracts Services

Property	1 3 7 8-TetraCDF	2,3,6,8-TetraCDF	2,3,7,8- TetraCDE	1,2,3,4,8-PentaCDF
Molecular weight	305.9	305.9	305.9	340.42
Color <sup>a</sup>	No data	Colorless <sup>b</sup>	Colorless	No data
Physical state <sup>c</sup>	Solid	Solid	Solid	Solid
Melting point, °C <sup>a</sup>	No data	197–198	219–221	177–178
Boiling point °C	No data	No data	No data	No data
Density at 20°C	No data	No data	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:	<b>N</b> <i>I I I I I I I I</i>	NI 17	<b>N</b> 1 1 <i>i</i>	<b>N</b> 1 1 <i>i</i>
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility: Water <sup>d</sup>	No data	No data	1.37x10 <sup>-9</sup> mol/L (0.43 µg/L)	No data
Organic solvents <sup>e</sup>	Soluble in toluene	Soluble in toluene and chloroform	Soluble in toluene	Soluble in toluene
Partition coefficients:				
Log K <sub>ow</sub> f	6.73	6.73	6.53	6.79
Log K <sub>oc</sub> h	No data	No data	5.61 (estimated)	No data
рКа	Not applicable	Not applicable	Not applicable	Not applicable
Vapor pressure at 25°C <sup>i</sup>	1.95x10 <sup>-8j</sup>	1.95x10 <sup>-8j</sup>	9.21x10 <sup>-7</sup>	No data
Henry's law constantk	1.48x10 <sup>-5</sup>	1.48x10 <sup>-5</sup>	1.48x10 <sup>-5</sup>	2.63x10 <sup>-5</sup>
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors Air <sup>a</sup> Water Soil	1 ppb = 12.72 μg/m <sup>3</sup> 1 ppb = 1 μg/L 1 ppb = 1 μg/kg	1 ppb = 12.72 μg/m <sup>3</sup> 1 ppb = 1 μg/L 1 ppb = 1 μg/kg	1 ppb = 12.72 μg/m <sup>3</sup> 1 ppb = 1 μg/L 1 ppb = 1 μg/kg	1 ppb = 14.15 μg/m³ 1 ppb = 1 μg/L 1 ppb = 1 μg/kg
Explosive limits	No data	No data	No data	No data

Water14.15 $\mu$ g/m³14.15 $\mu$ g/m³15.58 $\mu$ g/m³1 ppb = 1 $\mu$ g/LSoil1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg			-		
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $	рКа	Not applicable	Not applicable	Not applicable	Not applicable
Autoignition temperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlammability limitsNo dataNo dataNo dataNo dataConversion factors Aira1 ppb =1 ppb =1 ppb =1 ppb =Water14.15 $\mu$ g/m314.15 $\mu$ g/m315.58 $\mu$ g/m31 ppb = 1 $\mu$ g/LSoil1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/kg		2.73x10 <sup>-7</sup>	1.63x10 <sup>-7</sup>	6.07x10 <sup>-8</sup>	6.07x10 <sup>-8</sup>
temperatureFlashpointNo dataNo dataNo dataNo dataFlammability limitsNo dataNo dataNo dataNo dataConversion factorsAira1 ppb =1 ppb =1 ppb =1 ppb =1 ppb =Water14.15 $\mu$ g/m³14.15 $\mu$ g/m³15.58 $\mu$ g/m³1 ppb = 1 $\mu$ g/LSoil1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/kg	Henry's law constantk	2.63x10 <sup>-5</sup>	2.63x10⁻⁵	2.78x10 <sup>-5</sup>	2.78x10 <sup>-5</sup>
Flammability limitsNo dataNo dataNo dataNo dataConversion factorsAira1 ppb =1 ppb =1 ppb =1 ppb =Water14.15 $\mu$ g/m³14.15 $\mu$ g/m³15.58 $\mu$ g/m³1 ppb = 1 $\mu$ g/LSoil1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg	0	No data	No data	No data	No data
Conversion factors   Air <sup>a</sup> 1 ppb =	Flashpoint	No data	No data	No data	No data
Aira1 ppb =1 ppb =1 ppb =1 ppb =1 ppb = 15.58 $\mu$ g/m³Water14.15 $\mu$ g/m³14.15 $\mu$ g/m³15.58 $\mu$ g/m³1 ppb = 1 $\mu$ g/LSoil1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg	Flammability limits	No data	No data	No data	No data
	Air <sup>a</sup> Water	14.15 μg/m³ 1 ppb = 1 μg/L	14.15 μg/m³ 1 ppb = 1 μg/L	15.58 μg/m³ 1 ppb = 1 μg/L	
Explosive infinits indicate indicate indicate indicate	Explosive limits	No data	No data	No data	No data

Molecular weight374.87374.87374.87409.31Color®No dataNo dataNo dataNo dataNo dataPhysical state®SolidSolidSolidSolidPhysical state®SolidSolidSolidSolidSolling point, °C®No dataNo dataNo dataNo dataDensity at 20°CNo dataNo dataNo dataNo dataNo dataDensity at 20°CNo dataNo dataNo dataNo dataNo dataOdorNo dataNo dataNo dataNo dataNo dataOdor threshold:WaterNo dataNo dataNo dataNo dataWaterNo dataNo dataNo dataNo dataNo dataSolubility:WaterdNo dataNo dataNo dataNo dataVaterd®No dataNo dataNo dataNo dataSoluble in tolueneCriganic solvents®Soluble in tolueneSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Log Kow <sup>4</sup> No dataNo dataNo dataNo dataLog Kow <sup>6</sup> No dataNo dataNo dataNo dataNo dataNo dataVapor pressure at 28°C'3.74x10-82.78x10-52.78x10-64.1x10-6AutognitionNo dataNo dataNo dataNo dataNo dataAutognitionNo dataNo dataNo dataNo dataNo dataIsshpointNo dataNo dataNo data <th></th> <th></th> <th></th> <th></th> <th></th>					
Color*No dataNo dataNo dataNo dataNo dataPhysical state°SolidSolidSolidSolidSolidPhysical state°SolidNo data180–181239–240236–237Boiling point, °CNo dataNo dataNo dataNo dataNo dataDensity at 20°CNo dataNo dataNo dataNo dataNo dataDdorNo dataNo dataNo dataNo dataNo dataAirNo dataNo dataNo dataNo dataNo dataSolubility:WaterdNo dataNo dataNo dataSoluble in tolueneVagendric coefficients:Soluble in tolueneSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Log Kon <sup>4</sup> No dataNo dataNo dataNo dataLog Kon <sup>4</sup> No dataNo dataNo dataNo dataNo dataVapor pressure at 25°Ci3.74x10-81.68x10-81.68x10-8Henry's law constant*2.78x10-52.78x10-54.1x10-6Autoignition emperatureNo dataNo dataNo data <td>Property</td> <td></td> <td></td> <td></td> <td></td>	Property				
Physical stateSolidSolidSolidSolidPhysical stateSolidSolidSolidSolidWetting point, °CNo dataNo dataNo dataNo dataDensity at 20°CNo dataNo dataNo dataNo dataDensity at 20°CNo dataNo dataNo dataNo dataDensity at 20°CNo dataNo dataNo dataNo dataDdorNo dataNo dataNo dataNo dataDdorNo dataNo dataNo dataNo dataOdorNo dataNo dataNo dataNo dataDdorNo dataNo dataNo dataNo dataOdorNo dataNo dataNo dataNo dataDdorNo dataNo dataNo dataNo dataOdorNo dataNo dataNo dataNo dataSolubility:WaterNo dataNo dataNo dataWater <sup>d</sup> No dataNo dataNo dataSoluble in toluenePartition coefficients:Log Kow <sup>f</sup> No dataNo dataNo dataLog Kow <sup>f</sup> No dataNo dataNo dataNo dataNo dataDKaNot applicableNot applicableNot applicableNot applicableVapor pressure at 25°Ci3.74x10-52.78x10-52.78x10-54.1x10-6AutoignitionNo dataNo dataNo dataNo dataPany's law constant <sup>6</sup> 2.78x10-52.78x10-52.78x10-54.1x10-6Conversion factors	Molecular weight	374.87	374.87	374.87	409.31
Welting point, °C*No data180–181239–240236–2373oiling point, °CNo dataNo dataNo dataNo dataNo dataDensity at 20°CNo dataNo dataNo dataNo dataNo dataOdorNo dataNo dataNo dataNo dataNo dataNo dataOdorNo dataNo dataNo dataNo dataNo dataNo dataOdor threshold:WaterNo dataNo dataNo dataNo dataNo dataOdor threshold:WaterNo dataNo dataNo dataNo dataNo dataSolubility:WaterdNo dataNo dataNo dataNo dataSoluble in tolueneOrganic solvents*Soluble in tolueneSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Log Kow!No dataNo dataNo dataNo dataLog Kow!No dataNo dataNo dataNo dataNo dataSolaNot applicableNot applicableNot applicableNot applicableVapor pressure at 25°Ci3.74x10-82.78x10-52.78x10-64.1x10-6AutoignitionNo dataNo dataNo dataNo dataNo dataPanyo if the subjectiveNo dataNo dataNo dataNo dataCirc Kow!No dataNo dataNo dataNo dataNo dataLog Kow!No dataNo dataNo dataNo dataNo dataLog Kow!No dataNo dataNo	Color <sup>a</sup>	No data	No data	No data	No data
Boiling point, °CNo dataNo dataNo dataNo dataDensity at 20°CNo dataNo dataNo dataNo dataNo dataDdorNo dataNo dataNo dataNo dataNo dataDdorNo dataNo dataNo dataNo dataNo dataDdor threshold:WaterNo dataNo dataNo dataNo dataWaterNo dataNo dataNo dataNo dataNo dataSolubility:WaterdNo dataNo dataNo data3.31x10 <sup>-12</sup> mol/L (0.014 µg/L)Organic solventseSoluble in tolueneSoluble in tolueneSoluble in soluble in tolueneSoluble in toluenePartition coefficients:Log KowfNo dataNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataNo dataNo dataVapor pressure at 25°C3.74x10-83.74x10-81.68x10-82.78x10-54.1x10-8Autoignition emperatureNo dataNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataNo dataConversion factors Aira*1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/LSoil1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L	Physical state <sup>c</sup>	Solid	Solid	Solid	Solid
Density at 20°C No data No data No data No data No data Density at 20°C No data No data No data No data No data Dodor Mo data No data No data No data No data Mater No data No data No data No data Solubility: Water No data No data No data No data No data Solubility: Water No data No data No data No data Solubility: Water No data No data No data No data Soluble in toluene Soluble in toluene Soluble in toluene Partition coefficients: Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data No data No data No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data No data No data No data No data No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data Log K <sub>ow</sub> <sup>f</sup> No data No data No data No data No data No data No data No data No data No data No data No data No data Autoignition No data No data No data Conversion factors Air <sup>a</sup> 1 ppb = 1 pg/L 1 ppb = 1 µg/Kg 1 ppb	Melting point, °Cª	No data	180–181	239–240	236–237
DdorNo dataNo dataNo dataNo dataNo dataDdor threshold:WaterNo dataNo dataNo dataNo dataAirNo dataNo dataNo dataNo dataNo dataSolubility:WaterdNo dataNo dataNo data $3.31 \times 10^{-12} \text{ mol/L} (0.014 \ \mug/L)$ Organic solventseSoluble in tolueneSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Soluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:No dataNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataNo dataDXaNo dataNo dataNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataNo dataVator pressure at 25°Ci2.78x10-52.78x10-54.1x10-8Henry's law constantk2.78x10-52.78x10-54.1x10-8AutoignitionNo dataNo dataNo data <t< td=""><td>Boiling point, °C</td><td>No data</td><td>No data</td><td>No data</td><td>No data</td></t<>	Boiling point, °C	No data	No data	No data	No data
DeferminantNo dataNo dataNo dataNo dataWaterNo dataNo dataNo dataNo dataNo dataAirNo dataNo dataNo dataNo dataNo dataSolubility:WaterdNo dataNo dataNo data $3.31 \times 10^{-12} \text{ mol/L} (0.014 \ \mu g/L)$ Organic solvents®Soluble in tolueneSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Log KowfNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataNot applicableNot applicableNot applicableNot applicableVapor pressure at 25°Ci3.74x10-81.68x10-8Henry's law constant*2.78x10-52.78x10-54.1x10-6AutoignitionNo dataNo dataNo dataNo dataConversion factorsIppb = 1 ppb = 1 pg/L1 ppb = 1 µg/L1 ppb = 1 µg/LSoil1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/LSoil1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L	Density at 20°C	No data	No data	No data	No data
WaterNo dataNo dataNo dataNo dataNo dataAirNo dataNo dataNo dataNo dataNo dataSolubility:WaterdNo dataNo dataNo data $3.31 \times 10^{-12} \text{ mol/L} (0.014 \ \mu g/L)$ Organic solventseSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Soluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:No dataNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataNo dataVapor pressure at $2.74 \times 10^{-8}$ $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ AutoignitionNo dataNo dataNo dataNo dataNo dataemperature	Odor	No data	No data	No data	No data
AirNo dataNo dataNo dataNo dataSolubility:WaterdNo dataNo data $3.31 \times 10^{-12} \text{ mol/L} (0.014 \ \mu g/L)$ Organic solventseSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Soluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:No dataNo dataNo dataNo dataLog KowfNo dataNo dataJAKaNot applicableNot applicableNot applicableNot applicableVapor pressure at $3.74 \times 10^{-8}$ $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ Henry's law constantk $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ No dataFlashpointNo dataNo dataNo dataNo dataConversion factorsIppb = 1 ppb =1 ppb =1 ppb = 1 pp/LAira1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/LSoil1 ppb = 1 µg/L1 ppb = 1 µg/L	Odor threshold:				
Solubility:No dataNo dataNo dataNo data $3.31 \times 10^{-12} \text{ mol/L}$ (0.014 µg/L)Organic solvents®Soluble in tolueneSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Log KowfNo dataNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataNo dataJapor pressure at 25°Ci $3.74 \times 10^{-8}$ $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ Autoignition emperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataConversion factors Aira1 ppb =1 ppb =1 ppb =1 ppb =Aira1 ppb =1 ppb =1 ppb =1 ppb =1 ppb =Soil1 ppb =1 µg/L1 ppb =1 µg/L1 ppb =1 µg/kg	Water	No data	No data	No data	No data
WaterdNo dataNo dataNo dataNo data $3.31 \times 10^{-12} \text{ mol/L} (0.014 \ \mu g/L)$ Organic solventseSoluble in tolueneSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Log KowfNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataLog KochNo dataNo dataNo dataNo dataVapor pressure at 25°Ci $3.74 \times 10^{-8}$ No data $3.74 \times 10^{-8}$ Henry's law constantk $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ Autoignition emperatureNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataNo dataNo dataNo dataConversion factors Aira1 ppb = 1 pg/L 1 ppb = 1 µg/L1 ppb = 1 µg/L 1 ppb = 1 µg/L1 ppb = 1 µg/L 1 ppb = 1 µg/kg	Air	No data	No data	No data	No data
Organic solventseSoluble in tolueneSoluble in tolueneSoluble in tolueneSoluble in toluenePartition coefficients:Log KowfNo dataNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataNo dataLog KochNo dataNo dataNo dataNo dataNo dataVapor pressure at 25°Ci $3.74 \times 10^{-6}$ $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ Henry's law constantk $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ Autoignition emperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataConversion factors Aira1 ppb = 1 pg/L1 ppb = 1 pg/L1 ppb = 1 pg/LNoble = 1 pg/L 1 ppb = 1 pg/Kg1 ppb = 1 pg/Kg1 ppb = 1 pg/Kg1 ppb = 1 pg/Kg	Solubility:				
toluenePartition coefficients:Log KowfNo dataNo dataNo dataNo dataLog KowfNo dataNo dataNo dataNo dataNo dataLog KochNo dataNo dataNo dataNo dataNo dataoKaNot applicableNot applicableNot applicableNot applicableVapor pressure at 25°Ci $3.74 \times 10^{-8}$ No data $3.74 \times 10^{-8}$ $1.68 \times 10^{-8}$ Henry's law constant* $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ Autoignition emperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlammability limitsNo dataNo dataNo dataNo dataConversion factors Aira1 ppb =1 ppb =1 ppb =1 ppb =Aira1 ppb =1 ppb =1 ppb =1 ppb =1 ppb =Soil1 ppb =1 µg/L1 ppb =1 ppb =1 µg/L1 ppb =1 µg/kg1 ppb =1 µg/kg1 ppb =1 µg/kg	Water <sup>d</sup>	No data	No data	No data	••••
Log KowfNo dataNo dataNo dataNo dataNo dataLog KowfNo dataNo dataoKaNot applicableNot applicableNot applicableNot applicableVapor pressure at 25°Ci $3.74 \times 10^{-8}$ No data $3.74 \times 10^{-8}$ $1.68 \times 10^{-8}$ Henry's law constantk $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ Autoignition remperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataConversion factors Aira1 ppb =1 ppb =1 ppb =1 ppb = 17.02 µg/m³Aira1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/LSoil1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L	Organic solvents <sup>e</sup>	Soluble in toluene	Soluble in toluene		Soluble in toluene
Log KochNo dataNo dataNo dataNo dataNo dataOKaNot applicableNot applicableNot applicableNot applicableNot applicableVapor pressure at 25°Ci $3.74 \times 10^{-8}$ $3.74 \times 10^{-8}$ $1.68 \times 10^{-8}$ Henry's law constant* $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ AutoignitionNo dataNo dataNo dataNo dataemperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataConversion factorsAira1 ppb =1 ppb =1 ppb =Aira1 ppb =1 ppb =1 ppb =1 ppb =Soil1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/L1 ppb = 1 µg/kg1 ppb = 1 µg/kg1 ppb = 1 µg/kg	Partition coefficients:				
bKaNot applicableNot applicableNot applicableNot applicableNot applicableVapor pressure at 25°Ci $3.74 \times 10^{-8}$ $3.74 \times 10^{-8}$ $1.68 \times 10^{-8}$ Henry's law constant* $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ Autoignition remperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataConversion factors Water $1.558 \ \mu g/m^3$ $15.58 \ \mu g/m^3$ $15.58 \ \mu g/m^3$ $15.58 \ \mu g/m^3$ Soil $1 \ ppb = 1 \ \mu g/L$ $1 \ ppb = 1 \ \mu g/kg$ $1 \ ppb = 1 \ \mu g/kg$ $1 \ ppb = 1 \ \mu g/kg$	Log K <sub>ow</sub> f	No data	No data	No data	No data
Vapor pressure at 25°Ci $3.74 \times 10^{-8}$ No data $3.74 \times 10^{-8}$ $1.68 \times 10^{-8}$ Henry's law constantk 2.78x10^{-5} $2.78 \times 10^{-5}$ $2.78 \times 10^{-5}$ $4.1 \times 10^{-6}$ Autoignition emperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlammability limitsNo dataNo dataNo dataNo dataConversion factors Mater1 ppb =1 ppb =1 ppb =1 ppb =Aira1 ppb =1 ppb =1 ppb =1 ppb =1 ppb =Soil1 ppb = 1 µg/L 1 ppb = 1 µg/kg1 ppb =1 µg/L 1 ppb =1 ppb =1 ppb =1 µg/kg	Log K <sub>oc</sub> h	No data	No data	No data	No data
25°CiHenry's law constantk2.78x10-52.78x10-52.78x10-54.1x10-6Autoignition temperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataConversion factorsAira1 ppb =1 ppb =1 ppb =1 ppb =Water15.58 µg/m315.58 µg/m315.58 µg/m315.58 µg/m31 ppb =1 ppb =Soil1 ppb = 1 µg/L1 ppb =1 ppb =1 ppb =1 µg/L1 ppb =1 µg/L1 ppb =1 µg/L1 ppb =1 µg/LNoil1 ppb =1 µg/L1 ppb =1 µg/L1 ppb =Year1 ppb =1 µg/L1 ppb =1 µg/LYear1 ppb = <td>pKa</td> <td>Not applicable</td> <td>Not applicable</td> <td>Not applicable</td> <td>Not applicable</td>	pKa	Not applicable	Not applicable	Not applicable	Not applicable
Autoignition temperatureNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlashpointNo dataNo dataNo dataNo dataFlammability limitsNo dataNo dataNo dataNo dataConversion factorsAir <sup>a</sup> 1 ppb =1 ppb =1 ppb =Aira1 5.58 $\mu$ g/m <sup>3</sup> 15.58 $\mu$ g/m <sup>3</sup> 15.58 $\mu$ g/m <sup>3</sup> 15.58 $\mu$ g/m <sup>3</sup> Soil1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg	Vapor pressure at 25°C <sup>i</sup>	3.74x10 <sup>-8</sup>	No data	3.74x10 <sup>-8</sup>	1.68x10 <sup>-8</sup>
International internation of the target internation of ta	Henry's law constant <sup>k</sup>	2.78x10 <sup>-5</sup>	2.78x10 <sup>-5</sup>	2.78x10 <sup>-5</sup>	4.1x10 <sup>-6</sup>
Flammability limitsNo dataNo dataNo dataNo dataConversion factorsAir <sup>a</sup> 1 ppb =1 ppb =1 ppb =1 ppb =1 ppb =Water15.58 $\mu$ g/m <sup>3</sup> 15.58 $\mu$ g/m <sup>3</sup> 15.58 $\mu$ g/m <sup>3</sup> 1 ppb = 1 $\mu$ g/LSoil1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/kg	Autoignition temperature	No data	No data	No data	No data
Conversion factors   Air <sup>a</sup> 1 ppb =	Flashpoint	No data	No data	No data	No data
Aira1 ppb =1 ppb =1 ppb =1 ppb =1 ppb =1 ppb = 17.02 $\mu$ g/m³Water15.58 $\mu$ g/m³15.58 $\mu$ g/m³15.58 $\mu$ g/m³1 ppb = 1 $\mu$ g/LSoil1 ppb = 1 $\mu$ g/L1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg1 ppb = 1 $\mu$ g/kg	Flammability limits	No data	No data	No data	No data
	Water	15.58 μg/m³ 1 ppb = 1 μg/L	15.58 μg/m³ 1 ppb = 1 μg/L	15.58 μg/m³ 1 ppb = 1 μg/L	
	Explosive limits				No data

Property	1,2,3,4,6,7,9- HeptaCDF	1,2,3,4,6,8,9- HeptaCDF	1,2,3,4,7,8,9- HeptaCDF	1,2,3,4,6,7,8,9- OctaCDF
Molecular weight	409.31	409.31	409.31	443.76
Color <sup>a</sup>	No data	No data	No data	No data
Physical state <sup>c</sup>	Solid	Solid	Solid	Solid
Melting point, °C <sup>a</sup>	No data	211–212	212–223	25°
Boiling point, °C	No data	No data	No data	537°
Density at 20°C	No data	No data	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water <sup>d</sup>	No data	No data	No data	2.61x10 <sup>-12</sup> mol/L (0.0012 μg/L) (3.0 μg/L) <sup>ι</sup>
Organic solvents <sup>e</sup>	Soluble in toluene	Soluble in toluene	Soluble in toluene	Soluble in toluene
Partition coefficients:				
Log K <sub>ow</sub> <sup>f</sup>	No data	No data	No data	8.20 (7.97) <sup>i</sup>
Log K <sub>oc</sub> <sup>h</sup>	No data	No data	No data	8.57 (estimated)
pKa	Not applicable	Not applicable	Not applicable	Not applicable
Vapor pressure at 25°C <sup>i</sup>	No data	No data	9.79x10 <sup>-9</sup>	No data
Henry's law constant <sup>k</sup>	4.1x10 <sup>-6</sup>	4.1x10 <sup>-6</sup>	4.1x10 <sup>-6</sup>	1.7x10 <sup>-6</sup>
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors Airª Water Soil	1 ppb = 17.02 µg/m <sup>3</sup> 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 17.02 µg/m <sup>3</sup> 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 17.02 μg/m <sup>3</sup> 1 ppb = 1 μg/L 1 ppb = 1 μg/kg	1 ppb = 18.45 μg/m <sup>3</sup> 1 ppb = 1 μg/L 1 ppb = 1 μg/kg

Property	1,2,3,4,6,7,9-	1,2,3,4,6,8,9-	1,2,3,4,7,8,9-	1,2,3,4,6,7,8,9-
	HeptaCDF	HeptaCDF	HeptaCDF	OctaCDF
Explosive limits	No data	No data	No data	No data

<sup>a</sup>Kuroki et al. 1984 unless otherwise stated.

<sup>b</sup>The polychlorinated dibenzofurans are present predominantly in the particulate phase in ambient air (Hunt and Maisel 1990).

°WHO 2000.

<sup>d</sup>Friesen et al. 1990 unless otherwise stated.

<sup>e</sup>Ryan et al. 1991 unless otherwise stated.

<sup>f</sup>Sijm et al. 1989 unless otherwise stated; some of the values are for two isomers that could not be separated. <sup>g</sup>Burkhard and Kuehl 1986.

<sup>h</sup>EPA 1985.

Eitzer and Hites 1988.

<sup>j</sup>Rordorf 1989.

<sup>k</sup>Eitzer and Hites 1989a; the values are for unseparated isomers of each homologous series.

<sup>I</sup>Frank and Schrap 1990.