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2021

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4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Dichlorobenzenes (DCBs) are chlorinated aromatic compounds. 1,2-DCB is used primarily as a precursor for 3,4-dichloroaniline herbicides (CMR 1996). 1,3-DCB is used in the production of various herbicides, insecticides, pharmaceuticals, and dyes (Krishnamurti 2001). 1,4-DCB is used as a deodorant for restrooms (Howard 1989), for moth control (O'Neil 2001), and as an insecticide (Farm Chemicals Handbook 1983). Information regarding the chemical identity of 1,2-, 1,3-, and 1,4-DCB is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The dichlorobenzene isomers, 1,2-DCB and 1,3-DCB, are colorless volatile liquids at room temperature (EPA 1985a). 1,2-DCB has a pleasant odor, while the odor of 1,3-DCB is unspecified (EPA 1985a; NIOSH 2005). 1, 4-DCB is a combustible crystalline solid that tends to sublime at ordinary room temperatures. It possesses a distinctive odor reportable to be noticeable at airborne concentrations between 30 and 60 ppm (by weight [ppm-w] or by volume [ppm-v] not specified; presumably "ppm" would refer to ppm by weight). Information regarding the physical and chemical properties of 1,2-, 1,3-, and 1,4-DCB is located in Table 4-2.

Table 4-1. Chemical Identity of 1,2-, 1,3-, and 1,4-Dichlorobenzene

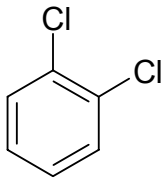
Characteristic	Value	Reference
Chemical name	1,2-Dichlorobenzene	Lide 2000
Synonyms	o-Dichlorobenzene; o-dichlorobenzol; orthodichlorobenzene	RTECS 2005
Trade names	Chloroben; Cloroben; Dilatin DB; Dowtherm E; Dizene; Special termite fluid; Termitkil	HSDB 2005; RTECS 2005
Chemical formula	$C_6H_4Cl_2$	RTECS 2005
Chemical structure		
Identification numbers:		
CAS Registry	95-50-1	Lide 2000
NIOSH RTECS	CZ4500000	RTECS 2005
EPA Hazardous Waste	U070; F002	HSDB 2005
OHM/TADS	No data	
DOT/UN/NA/IMCO Shipping	UN 1591; IMO 6.1	HSDB 2005
HSDB	521	HSDB 2005
NCI	NCI-C54944	RTECS 2005

Table 4-1. Chemical Identity of 1,2-, 1,3-, and 1,4-Dichlorobenzene

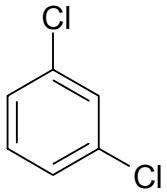
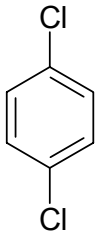
Characteristic	Value	Reference
Chemical name	1,3-Dichlorobenzene	Lide 2000; HSDB 2005
Synonyms	m-Dichlorobenzene; m-DCB; m-dichlorobenzol; m-phenylene dichloride	RTECS 2005
Trade names	No data	
Chemical formula	$C_6H_4Cl_2$	RTECS 2005
Chemical structure		
Identification numbers:		
CAS Registry	541-73-1	Lide 2000
NIOSH RTECS	CZ4499000	RTECS 2005
EPA Hazardous Waste	U071	HSDB 2005
OHM/TADS	No data	
DOT/UN/NA/IMCO Shipping	No data	
HSDB	522	HSDB 2005
NCI	No data	

Table 4-1. Chemical Identity of 1,2-, 1,3-, and 1,4-Dichlorobenzene

Characteristic	Value	Reference
Chemical name	1,4-Dichlorobenzene	Lide 2000
Synonyms	para-Dichlorobenzene; p-dichloro-benzene; p-chlorophenyl chloride; PDB; PDCB; p-dichlorobenzol	RTECS 2005
Trade names	Paracide; Paradow; Paradi; Santochlor; Paramoth; Paranuggets; Parazene; Persia-perazol; Para crystals; Global; Evola; Di-chloricide	RTECS 2005
Chemical formula	$C_6H_4Cl_2$	RTECS 2005
Chemical structure		
Identification numbers:		
CAS Registry	106-46-7	Lide 2000
NIOSH RTECS	CZ4550000	RTECS 2005
EPA Hazardous Waste	U072; D027	HSDB 2005
OHM/TADS	No data	
DOT/UN/NA/IMCO Shipping	UN 1592; IMO 6.1	HSDB 2005
HSDB	523	HSDB 2005
NCI	NCI-C54955	RTECS 2005

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/Intergovernmental 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 4-2. Physical and Chemical Properties of 1,2-, 1,3-, and 1,4-Dichlorobenzene

Property	Value	Reference
Chemical name	1,2-Dichlorobenzene	Lide 2000
Molecular weight	147.00	Lide 2000
Color	Colorless to pale yellow	NIOSH 2005
Physical state	Liquid	Lewis 1997
Melting point	-16.7 °C	Lide 2000
Boiling point	180 °C	Lide 2000
Density at 20 °C	1.3059 g/mL	Lide 2000
Odor	Pleasant, aromatic	NIOSH 2005
Odor threshold:		
Water	0.01 mg/L	Verschueren 2001
Air	50 ppm (301 mg/m^3)	Verschueren 2001
Solubility:		
Water	156 mg/L at 25 °C	Banerjee et al. 1980
Organic solvents	Miscible with alcohol, ether, benzene	O'Neil 2001
Partition coefficients:		
Log octanol/water	3.43	Hansch et al. 1995
Log K_{oc}	2.51	Chiou et al. 1983
Vapor pressure at 25 °C	1.36 mm Hg	Daubert and Danner 1992
Henry's law constant at 25 °C	1.92×10^{-3} atm m^3/mol	Shiu and Mackay 1997
Autoignition temperature	640 °C	Krishnamurti 2001
Flashpoint	28 °C (closed cup)	Krishnamurti 2001
Flammability limits	No data	
Conversion factors	1 mg/m^3=0.116 ppm at 25 °C and 760 mm Hg; 1 ppm=6.01 mg/m^3 at 25 °C and 760 mm Hg	Verschueren 2001
Explosion limits	2–9% by volume in air	Leber and Bus 2001

Table 4-2. Physical and Chemical Properties of 1,2-, 1,3-, and 1,4-Dichlorobenzene

Property	Value	Reference
Chemical name	1,3-Dichlorobenzene	Lide 2000
Molecular weight	147.00	Lide 2000
Color	Colorless	Lewis 1997
Physical state	Liquid	Lewis 1997
Melting point	-24.8 °C	Lide 2000
Boiling point	173 °C	Lide 2000
Density at 20 °C	1.2884 g/mL	Lide 2000
Odor	No data	
Odor threshold:		
Water	0.02 mg/L	Verschueren 2001
Air	No data	
Solubility:		
Water	125 mg/L at 20 °C	Miller et al. 1984
Organic solvents	Soluble in alcohol, ether	O'Neil 2001
Partition coefficients:		
Log octanol/water	3.53	Hansch et al. 1995
Log K_{oc}	2.47	Chiou et al. 1983
Vapor pressure at 25 °C	2.15 mm Hg	Daubert and Danner 1992
Henry's law constant at 25 °C	$2.8x10^{-3}$ atm m^3/mol	Staudinger and Roberts 1996
Autoignition temperature	>500 °C	Krishnamurti 2001
Flashpoint	No data	
Flammability limits	No data	
Conversion factors	1 mg/ m^3=0.116 ppm at 25 °C and 760 mm Hg; 1 ppm=6.01 mg/m^3 at 25 °C and 760 mm Hg	HSDB 2005
Explosion limits	No data	

Table 4-2. Physical and Chemical Properties of 1,2-, 1,3-, and 1,4-Dichlorobenzene

Property	Value	Reference
Chemical name	1,4-Dichlorobenzene	Lide 2000
Molecular weight	147.00	Lide 2000
Color	Colorless or white	NIOSH 2005
Physical state	Solid	Lewis 1997
Melting point	52.7 °C	Lide 2000
Boiling point	174 °C	Lide 2000
Density at 20 °C	1.46 g/mL	O'Neil 2001
Odor	Mothball-like; penetrating	Lewis 1997; NIOSH 2005
Odor threshold:		
Water	0.011 mg/L	Amoore and Hautala 1983
Air	0.18 ppm (1.1 mg/m^3)	Amoore and Hautala 1983
Solubility:		
Water	80.0 mg/L	Yalkowsky and He 2003
Organic solvents	Soluble in alcohol, ether, benzene, chloroform, carbon disulfide	O'Neil 2001
Partition coefficients:		
Log octanol/water	3.44	Hansch et al. 1995
Log K_{oc}	2.44	Chiou et al. 1983
Vapor pressure at 25 °C	1.77 mm Hg	Daubert and Danner 1992
Henry's law constant at 25 °C	2.41×10^{-3} atm m^3/mol	Shiu and Mackay 1997
Autoignition temperature	>500 °C	Krishnamurti 2001
Flashpoint	67 °C (closed cup)	Krishnamurti 2001
Flammability limits	6.2–16%	Leber and Bus 2001
Conversion factors	1 ppm=6.01 mg/m^3 at 25 °C and 760 mm Hg; 1 mg/m^3=0.166 ppm at 25 °C and 760 mm Hg	Verschueren 2001
Explosion limits	No data	