

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of 1,2-dibromo-3-chloropropane are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of 1,2-dibromo-3-chloropropane are presented in Table 3-2.

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of 1,2-Dibromo-3-chloropropane

Characteristic	Information	Reference
Chemical name	1,2-Dibromo-3-chloropropane	CAS 1989
Synonyms	DBCP; BBC12	CAS 1989
Trade names	Nemagon; Nemaforme; Fumazone; Fumagon; Nemabrom; Nemazon; OS 1897; and others	OHM/TADS 1989
Chemical formula	$C_3H_5Br_2Cl$	CAS 1989
Chemical structure	$ \begin{array}{c} CH_2CHCH_2 \\ \quad \quad \backslash \\ Br \quad Br \quad Cl \end{array} $	CAS 1989
Identification numbers:		
CAS registry	96-12-8	CAS 1989
NIOSH RTECS	TX8750000	HSDB 1989
EPA hazardous waste	U066	HSDB 1989
OHM/TADS	7216513	OHM/TADS 1989
DOT/UN/NA/IMCO shipping	UN 2872	HSDB 1989
HSDB	1629	HSDB 1989
NCI	C00500	HSDB 1989

CAS = Chemical Abstracts Service; EPA = Environmental Protection Agency;
 DOT/UN/NA/IMCO = Department of Transportation/ United Nations/ North America/
 International Maritime Dangerous Goods Code; 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

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-2. Physical and Chemical Properties of 1,2-Dibromo-3-chloropropane

Property	Information	Reference
Molecular weight	236.36	Windholz 1983
Color	Colorless (when pure); amber to dark brown, yellow (technical grade)	Sax and Lewis 1987; Verschuieren 1983; NIOSH 1985
Physical state	Liquid	Windholz 1983
Melting point	6°C	Stenger 1978
Boiling point	196°C	Windholz 1983
Density at 14°C	2.093 g/cm ³	Windholz 1983
Odor	Pungent	Windholz 1983
Odor threshold:		
Water	No data	
Air	0.0965 mg/m ³	Ruth 1986
Solubility:		
Water at 20°C	1,230 mg/L	Munnecke and VanGundy 1979
Organic solvents	Miscible with methanol, ethanol, isopropyl alcohol, hydrocarbons, halogenated hydrocarbons, and oils	IARC 1979; Windholz 1983
Partition coefficients:		
Log K _{ow}	2.26 (estimated)	EPA 1988a
Log K _{oc}	2.17; 2.11	Sabljić 1984; Wilson et al. 1981
Bioconcentration factor	11.2 ^a	Bysshe 1982
Vapor pressure at 20°C	0.58 mmHg	Munnecke and VanGundy 1979
Henry's law constant:		
at 20°C	1.47x10 ⁻⁴ atm-m ³ /mol ^b	Thomas 1982
Autoignition temperature	No data	
Flashpoint:		
Open cup	76.6°C (170°F)	Sax and Lewis 1987
Flammability limits	No data	

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-2 (Continued)

Property	Information	Reference
Conversion factors:		
ppm (v/v) to mg/m ³ in air (20°C)	1 ppm (v/v) x 9.67 = mg/m ³	
mg/m ³ to ppm (v/v) in air (20°C)	1 mg/m ³ x 0.103 = ppm (v/v)	
Explosive limits	No data	

^aCalculated from water solubility using equation 5-3 in Lyman et al. 1982

^bCalculated from vapor pressure and water solubility using equation 15-8 in Lyman et al. 1982