

CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of 1,2-dibromo-3-chloropropane are listed in Table 4-1.

Table 4-1. Chemical Identity of 1,2-Dibromo-3-Chloropropane

Characteristic	Information	Reference
Chemical name	1,2-Dibromo-3-chloropropane	CAS 1989
Synonym(s) and registered trade name(s)	Nemagon; Nemaflume; Fumazone; Fumagon; Nemabrom; Nemazon; OS 1897; and others	OHM/TADS 1989
Chemical formula	C ₃ H ₅ Br ₂ Cl	CAS 1989
Chemical structure	$ \begin{array}{c} \text{H} \quad \text{H}_2 \\ \quad \\ \text{H}_2\text{C}-\text{C}-\text{C} \\ \quad \quad \\ \text{Br} \quad \text{Br} \quad \text{Cl} \end{array} $	CAS 1989
CAS Registry Number	96-12-8	CAS 1989

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of 1,2-dibromo-3-chloropropane are presented in Table 4-2.

Table 4-2. 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)	NIOSH 1985; Sax and Lewis 1987; Verschueren 1983
Physical state	Liquid	Windholz 1983
Melting point	6°C	Stenger 1978
Boiling point	196°C	Windholz 1983
Density at 20°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

4. CHEMICAL AND PHYSICAL INFORMATION

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

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	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
Vapor pressure at 20°C	0.58 mmHg	Munnecke and VanGundy 1979
Henry's law constant at 25°C	1.47x10 ⁻⁴ atm-m ³ /mol ^a	Thomas 1982
Autoignition temperature	No data	
Flashpoint	76.6°C (open cup)	Sax and Lewis 1987
Flammability limits	No data	
Conversion factors	1 ppm=9.67 mg/m ³	
Explosive limits	No data	

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