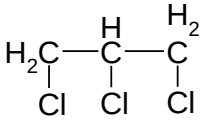
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

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

Table 4-1. Chemical Identity of 1,2,3-Trichloropropane

Characteristic	Information	Reference
Chemical name	1,2,3-Trichloropropane	NLM 2020
Synonym(s) and registered trade name(s)	Allyl trichloride; glycerol trichlorohydrin; trichlorohydrin	NLM 2020
Chemical formula	$C_3H_5Cl_3$	NLM 2020
Chemical structure		
CAS Registry Number	96-18-4	NLM 2020

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

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

Property	Information	Reference
Molecular weight	147.43	Weast 1985
Color	Colorless	Hawley 1981
Physical state	Liquid	Hawley 1981
Melting point	-14.7°C	Williams 1949
Boiling point	156.8°C	Riddick et al. 1986
Density at 20 °C	1.3888 g/cm^2	Riddick et al. 1986
Odor	Strong, acrid; trichloroethylene-like; “sweet smelling”	McNeill 1979; NLM 2020; Ruth 1986
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 20 °C	1,750 mg/L	Riddick et al. 1986
Organic solvents	Soluble in ethyl alcohol and higher alcohols, chloroform and other chlorinated hydrocarbons, ethyl ether, benzene	Weast 1985; Williams 1949
Partition coefficients:		
Log K_{ow}	2.27	NLM 2020
Log K_{oc}[a]	1.99 (estimated)	Lyman et al. 1982
Bioconcentration factor[b]	9.2 (estimated)	Lyman et al. 1982
Vapor pressure at 20°C	3.1 mmHg	Mackay et al. 1982
Henry's law constant at 25°C	3.17x10^{-4} atm-m^3/mol (calculated)	Lyman et al. 1982
Autoignition temperature	304°C (580°F)	Hawley 1981
Flashpoint		
Open cup	82.2°C	Hawley 1981
Open cup	78.9°C	Williams 1949
Closed cup	73.3°C	Williams 1949
Flammability limits	No data	
Conversion factors	1 ppm (v/v)x6.03 = mg/m^2 1 mg/m^{3}x0.166 = ppm (v/v)	
Explosive limits	No data	

[a]Calculated from water solubility using equation 4-7 (Lyman et al. 1982).
[b]Calculated from log K_{ow} using equation 5-2 (Lyman et al. 1982).