3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

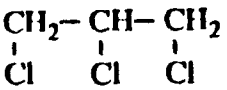
Data pertaining to the chemical identity of 1,2,3-trichloropropane are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

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

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of 1,2,3-Trichloropropane

Characteristic	Information	Reference
Chemical name	1,2,3-Trichloropropane	CAS 1989
Synonyms	Allyl trichloride; glycerol trichlorohydrin; trichlorohydrin	CAS 1989
Trade names	No data	
Chemical formula	$C_3H_5Cl_3$	CAS 1989
Chemical structure		
Identification numbers:		
CAS registry	96-18-4	CAS 1989
NIOSH RTECS	TZ9275000	RTECS 1989
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	No data	
HSDB	1340	CHEMLINE 1989
NCI	C60220	HSDB 1989
USDA	AI3-26040	CHEMLINE 1989

CAS = Chemical Abstracts Service
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
USDA = United States Department of Agriculture

TABLE 3-2. 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^3	Riddick et al. 1986
Dissociation constant at 25°C (pKa)	No data	
Odor	Strong, acrid; trichloroethylene-like: "sweet smelling"	Ruth 1986; HSDB 1989; McNeill 1979
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 20°C	1750 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 octanol/water	1.98	EPA 1988b
Log K_oc[a]	1.99 (estimated)	Lyman et al. 1982
Bioconcentration factor[b]	9.2 (estimated)	Lyman et al. 1982
Vapor pressure at 25°C	3.1 mmHg	Mackay et al. 1982
Henry's law constant: at 25°C[c]	3.17×10^{-4} atm-m3/mol (calculated)	Lyman et al. 1982
Autoignition temperature	304°C (580°F)	Hawley 1981
Flashpoint		
open cup	82.2°C (180°F)	Hawley 1981
open cup	78.9°C (174°F)	Williams 1949
closed cup	73.3°C (164°F)	Williams 1949

TABLE 3-2 (Continued)

Property	Information	Reference
Flammability limits	No data	
Conversion factors		
ppm (v/v) to mg/m^3 in air (20°C)	1 ppm (v/v)x6.03 = mg/m^3	
mg/m^3 to ppm (v/v) in air (20°C)	1 mg/m^3x0.166 = ppm (v/v)	
Explosive limits	No data	

[a]Calculated from water solubility using equation 4-7 (Lyman et al. 1982).
[b]Calculated $_f$rom from log K_ow using equation 5-2 (Lyman et al. 1982).
[c]Calculated from vapor pressure and water solubility using equation 15-8 (Lyman et al. 1982).