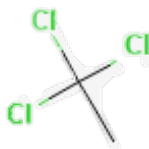


CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

1,1,1-Trichloroethane is a man-made chlorinated hydrocarbon chemical that was widely used as a solvent and in metal degreasing. It is a synthetic compound. U.S. production of 1,1,1- trichloroethane was to be cut incrementally as per Section 604 of the Clean Air Act and Montreal Protocol, eventually being completely phased out by January 2002, and cease production by 2012 as a result of ozone depletion agreements from the Montreal Protocol (Kapp 2014). While the Montreal Protocol reduced the production of 1,1,1-trichloroethane, some production does continue with a steady decline in the ambient air levels. Table 4-1 lists common synonyms, trade names, and other pertinent identification information for 1,1,1-trichloroethane.

Table 4-1. Chemical Identity of 1,1,1-Trichloroethane

Characteristic	Information	Reference
Chemical Name	1,1,1-Trichloroethane	HSDB 2015
Synonym(s) and Registered trade name(s)	Methylchloroform; Chloroethene; Chloroetene; Inhibisol; Aerothene MM; Aerothene TT; Solvent 111; Alpha T	HSDB 2015
Chemical formula	C ₂ H ₃ Cl ₃	Haynes et al. 2015
Chemical structure		PubChem 2022
CAS registry number	71-55-6	Haynes et al. 2015

CAS = Chemical Abstracts Service; HSDB = Hazardous Substances Data Bank

4.2 PHYSICAL AND CHEMICAL PROPERTIES

1,1,1-Trichloroethane is a volatile organic compound. It is slightly soluble in water, and the Henry's law constant suggests it is readily volatilized from water. Based on the log K_{ow} and log K_{oc} values, 1,1,1-trichloroethane is expected to have high mobility in soil. With a vapor pressure of 124 mm Hg at 25°C, 1,1,1-trichloroethane exists in the atmosphere in the vapor phase. Table 4-2 lists important physical and chemical properties of 1,1,1-trichloroethane.

4. CHEMICAL AND PHYSICAL INFORMATION

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

Property	Information	Reference
Molecular weight	133.4	Haynes et al. 2015
Color	Colorless	NIOSH 2019
Physical state	Liquid	Haynes et al. 2015
Melting point	-30°C	Haynes et al. 2015
Boiling point	74°C	Haynes et al. 2015
Density: At 20°C/4°C	1.3376	Haynes et al. 2015
Odor	Mild, chloroform-like	NIOSH 2019
Odor threshold:		
Water	No data	
Air	120 ppm 500 ppm	Amoore and Hautala 1983 Reist and Rex 1977
Taste threshold	No data	
Solubility:		
Water	1.29 g/L H ₂ O at 25°C; slightly soluble in H ₂ O	Haynes et al. 2015
Organic solvent(s)	Soluble in ethanol and chloroform, miscible in diethyl ether Soluble in acetone, benzene, methanol, carbon tetrachloride, and ether	O'Neil 2013
Partition coefficients:		
Log K _{ow}	2.49	Haynes et al. 2015
Log K _{oc}	2.03 2.02	Friesel et al. 1984 Chiou and Freed 1979
Vapor pressure At 20°C	16.5 kPa (123.8 mmHg) at 25°C	Haynes et al. 2015
Henry's law constant	0.0163 atm-cu m/mole at 25°C	Warneck 2007
Autoignition temperature	500°C	HSDB 2015
Flashpoint	>200°F	OSHA 2021
Conversion factors		
ppm (v/v) to mg/m ³ in air (20°C)	1 ppm = 5.46 mg/m ³	NIOSH 2019
mg/m ³ to ppm (v/v) in air (20°C)	1 mg/m ³ = 0.185 ppm	Chiou et al. 1980
Explosive limits	7.5–12.5% in air	NIOSH 2019

HSDB = Hazardous Substances Data Bank; NIOSH = National Institute for Occupational Safety and Health