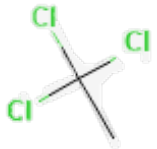
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

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. Information regarding the chemical identity of 1,1,1-trichloroethane is presented in Table 4-1.

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

Characteristic	Information	Reference
Chemical name	1,1,1-Trichloroethane	NLM 2023
Synonym(s) and registered trade name(s)	Methylchloroform; chlorothene; chloroetene; Inhibisol; Aerothene MM; Aerothene TT; Solvent 111; Alpha T	NLM 2022
Chemical formula	$C_2H_3Cl_3$	Haynes et al. 2015
SMILES	CC(Cl)(Cl)Cl	NLM 2023
Chemical structure		NLM 2023
CAS registry number	71-55-6	Haynes et al. 2015

CAS = Chemical Abstracts Service; SMILES = simplified molecular-input line-entry system

4.2 PHYSICAL AND CHEMICAL PROPERTIES

1,1,1-Trichloroethane is a volatile organic compound (VOC). It is slightly soluble in water, and its Henry's law constant suggests that 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. Information regarding physical and chemical properties of 1,1,1-trichloroethane is presented in Table 4-2.

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 Air	 No data 120 ppm 500 ppm	 Amoore and Hautala 1983; Reist and Rex 1977
Taste threshold	No data	
Solubility: Water at 25°C Organic solvent(s)	 1.29 g/L H_2O; slightly soluble in H_2O Soluble in ethanol and chloroform, miscible in diethyl ether; soluble in acetone, benzene, methanol, carbon tetrachloride, and ether	 Haynes et al. 2015; O'Neil 2013
Partition coefficients: Log K_{ow} Log K_{oc}	 2.49 2.03 2.02	 Haynes et al. 2015 Friesel et al. 1984 Chiou et al. 1979
Vapor pressure at 25°C	16.5 kPa (123.8 mmHg)	Haynes et al. 2015
Henry's law constant at 25°C	0.0163 atm-m^3/mole	Warneck 2007
Autoignition temperature	537°C	NLM 2023
Flashpoint	>200°F	NLM 2023
Conversion factors ppm (v/v) to mg/m^3 in air (20°C) mg/m^3 to ppm (v/v) in air (20°C)	 1 ppm = 5.46 mg/m^3 1 mg/m^3 = 0.185 ppm	 NIOSH 2019 Chiou et al. 1980
Explosive limits	7.5–12.5% in air	NIOSH 2019