

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

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

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 1,1,1-trichloroethane is located in Table 4-2.

4. CHEMICAL AND PHYSICAL INFORMATION

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

Characteristic	Information	Reference
Chemical name	1,1,1-Trichloroethane	CAS 2004
Synonyms(s)	Methylchloroform	CAS 2004
	Methyltrichloromethane	CAS 2004
	1,1,1-TCE	
	Trichloromethylmethane	
	α -Trichloromethane	
Registered trade name(s)	Chlorothene NU	OHM/TADS 1994
	Aerothene TT	
Chemical formula	CCl_3CH_3	CAS 2004
Chemical structure	$ \begin{array}{c} \text{Cl} \quad \text{H} \\ \quad \\ \text{Cl}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{Cl} \quad \text{H} \end{array} $	
Identification numbers:		
CAS registry	71-55-6	CAS 2004
NIOSH RTECS	KJ2975000	RTECS 2004
EPA hazardous waste	U226, F002	HSDB 2005
OHM/TADS	8100101	OHM/TADS 1994
DOT/UN/NA/IMCO shipping	UN 2831, IMO 6.1	HSDB 2005
HSDB	157	HSDB 2005
NCI	C04626	HSDB 2005

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; 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

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

Property	Information	Reference
Molecular weight	133.4	CAS 2004
Color	Colorless	Archer 1979; Sax and Lewis 1987
Physical state	Liquid	Merck 1989
Melting point	-30.4 °C -33.0 °C	Weast 1988 Archer 1979
Boiling point	74.1 °C	Budavari 1989
Density:		
at 20 °C	1.3390 g/mL	Weast 1988
at 25 °C	1.3299 g/mL	Riddick et al. 1986
at 30 °C	1.32096 g/mL	Riddick et al. 1986
Odor	Ethereal, chloroform-like	Archer 1979; Aviado et al. 1976
Odor threshold:		
Water	No data	
Air	120 ppm 500 ppm	Amoore and Hautala 1983; Reist and Rex 1977
Solubility:		
Water at 25 °C	0.1495% (w/w) (1,500 mg/L)	Horvath 1982
Organic solvent(s)	Soluble in alcohol, ether, chloroform; miscible with other chlorinated solvents, soluble in common organic solvents	Archer 1979; Weast 1988
Partition coefficients:		
Log K _{ow}	2.49	Hansch and Leo 1985
Log K _{oc}	2.03 2.02	Friesel et al. 1984 Chiou et al. 1979
Vapor pressure at 20 °C	124 mm Hg 16.4 kPa	Boublik et al. 1984 Riddick et al. 1986
Henry's law constant:		
at 20 °C	6.3x10 ⁻³ atm	Chiou et al. 1980
at 30 °C	17.2x10 ⁻³ atm	Gossett 1987
Autoignition temperature	537 °C	HSDB 2004
Flashpoint	None	Archer 1979
Flammability limits	8–10.5%	Archer 1979
Conversion factors:		
ppm (v/v) to mg/m ³ in air (20 °C)	1 ppm = 5.4 mg/m ³	Chiou et al. 1980
mg/m ³ to ppm (v/v) in air (20 °C)	1 mg/m ³ = 0.185 ppm	
Explosive limits	7.5–12.5% in air	NIOSH 1990

CAS = Chemical Abstracts Services; HSDB = Hazardous Substances Data Bank; NIOSH = National Institute for Occupational Safety and Health; v/v = volume by volume; wt/wt = weight by weight