

CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

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

Table 4-1. Chemical Identity of 1,1,2-Trichloroethane

Characteristic	Information	Reference
Chemical name	1,1,2-trichloroethane	CAS 1988
Synonym(s) and registered trade name(s)	Ethane trichloride; β -Trichloroethane; Vinyl trichloride; 1,2,2-Trichloroethane	CAS 1988; SANSS 1988
Chemical formula	β -T; Cement T-339	SANSS 1988
Chemical structure	$ \begin{array}{c} \text{Cl} \quad \text{H} \\ \quad \\ \text{Cl}-\text{C}-\text{C}-\text{Cl} \\ \quad \\ \text{H} \quad \text{H} \end{array} $	CAS 1988
Identification numbers:		
CAS Registry	79-00-5	CAS 1988

CAS = Chemical Abstracts Services

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

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

Property	Information	Reference
Molecular weight	133.41 g/mol	Riddick et al. 1986
Color	Colorless	Hawley 1981
Physical state	Liquid	Hawley 1981
Melting point	-36.53°C	Riddick et al. 1986
Boiling point	113.85°C	Riddick et al. 1986
Density at 20°C	1.43931 1.4416 1.443	Riddick et al. 1986 Torkelson and Rowe 1981 Windholz 1983
Odor	Sweet	Hawley 1981
Solubility:		
Water at 20°C	4,400 mg/L	Riddick et al. 1986
Organic solvents	Miscible with ethers, alcohols, esters, and ketones	Hawley 1981

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

Property	Information	Reference
Partition coefficients:		
Log K_{ow}	2.42	Isnard and Lambert 1988
Log K_{oc}	1.06–2.49 ^a (estimated)	Sabljić 1987
Vapor pressure at 25°C	22.49 mmHg	Riddick et al. 1986
Henry's law constant	9.1x10 ⁻⁴ atm/m ³ -mol (25°C) 1.12x10 ⁻³ atm/m ³ -mol (30°C) ^b	Ashworth et al. 1988
Autoignition temperature	460°C	Parrish 1983
Flashpoint	None	Hawley 1981
Flammability limits	8.4–13.3% (by volume)	Moolenaar and Olson 1989
Conversion factors:		
ppm (v/v) to mg/m ³ in air (20°C)	1 ppm (v/v) = 5.55 = mg/m ³	
mg/m ³ (v/v) to ppm in air (20°C)	1 mg/m ³ = 0.18 ppm (v/v)	

^aOrganic matter partition coefficient.

^bFirst value obtained using equilibrium partitioning in closed systems technique and second by the batch air-stripping method.