

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

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

3.2 PHYSICAL AND CHEMICAL PROPERTIES

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

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TABLE 3-1. Chemical Identity of 1,1,1-Trichloroethane

	Value	Reference
Chemical Name	1,1,2-Trichloroethane	CAS 1988
Synonyms	Ethane trichloride; β -Trichloroethane; Vinyl trichloride; 1,2,2-Trichloroethane	CAS 1988; SANSS 1988
Trade Name(s)	β -T; Cement T-339	SANSS 1988
Chemical Formula	C ₂ H ₃ Cl ₃	CAS 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} $	
Identification Numbers:		
CAS Registry	79-00-5	CAS 1988
NIOSH RTECS	KJ2975000	NLM 1988
EPA Hazardous Waste	U227	NLM 1988
OHM/TADS	8100016	OHMTADS 1988
DOT/UN/NA/IMCO Shipping	None	
HSDB	1412	NLM 1988
NCI	CO4579	RTECS 1988

CAS - Chemical Abstracts Services

NIOSH - National Institute for Occupational Safety and Health

RTECS - Registry of Toxic Effects of Chemical Substances

OHM/TADS - Oil and Hazardous Materials/Technical Assistance Data System

DOT/UN/NA/IMCO - Department of Transportation/United Nations/North America/
International Maritime Dangerous Goods Code

NLMS - National Library of Medicine

HSDB - Hazardous Substance Data Bank

NCI - National Cancer Institute

SANSS - Structure and Nomenclature Search System

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TABLE 3-2. Physical and Chemical Properties of 1,1,2-Trichloroethane

Property	Value	Reference
Molecular weight	133.41	Riddick et al. 1986
Color	Colorless	Hawley 1981
Physical state	Liquid	Hawley 1981
Freezing point	-36.53°C	Riddick et al. 1986
Boiling point	113.85°C	Riddick et al. 1986
Density, 20°C	1.43931	Riddick et al. 1986
20°C	1.4416	Merck 1983
20°C	1.443	Torkelson and Rowe 1981
Odor	Sweet	Hawley 1981
Odor threshold		
Water		
Air		
Solubility		
Water	4400 mg/L (20°C)	Riddick et al. 1986
Organic solvents	Miscible with ethers, alcohols, esters, and ketones	Hawley 1981
Partition coefficients		
Log octanol/water	2.42	Isnard and Lambert 1988
Log Koc	1.06-2.49 ^a (estimated)	Sabljić 1987
Vapor pressure	22.49 mm Hg (25°C)	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

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TABLE 3-2 (continued)

Property	Value	Reference
Flash point	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 to ppm (v/v) in air (20°C)	1 mg/m ³ = 0.18 ppm (v/v)	

^aOrganic matter partition function.

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