

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

The chemical formula, structure, synonyms, and identification numbers for 1,1-dichloroethene are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Important physical and chemical properties of 1,1-dichloroethene are listed in Table 3-2.

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

Characteristic	Information	Reference
Chemical name	1,1-Dichloroethene	HSDB 1992
Synonym(s)	DCE; 1,1-dichloroethylene; 1,1-DCE; asym-dichloroethylene; VDC; vinylidene chloride; vinylidene chloride (II); vinylidene dichloride; vinylidine chloride	HSDB 1992
Registered trade name(s)	No data	
Chemical formula	C ₂ H ₂ Cl ₂	Budavari 1989
Chemical structure	$\begin{array}{c} \text{Cl} - \text{C} = \text{C} - \text{H} \\ \quad \\ \text{Cl} \quad \text{H} \end{array}$	Budavari 1989
Identification numbers:		
CAS registry	75-35-4	HSDB 1992
NIOSH RTECS	KV9275000	HSDB 1992
EPA hazardous waste	U078/D029	HSDB 1992
OHM/TADS	7216949	HSDB 1992
DOT/UN/NA/IMCO shipping	UN 1303; IMO 3.1	HSDB 1992
HSDB	1995	HSDB 1992
NCI	C54262	HSDB 1992

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 3-2. Physical and Chemical Properties of 1,1-Dichloroethene

Property	Information	Reference
Molecular weight	96.95	Budavari 1989
Color	Colorless	Grayson 1985
Physical state	Liquid	Budavari 1989
Melting point, °C	-122.5	Budavari 1989
Boiling point, °C	31.7 at 760 mmHg	Budavari 1989
Density:		
at 20°C	1.213 g/cm ³	Budavari 1989
Odor	Mild sweet odor resembling that of chloroform	Budavari 1989
Odor threshold:		
Air	500 ppm	Torkelson and Rowe 1981
Solubility:		
Water at 25°C	2.5 g/L	HSDB 1992
Organic solvent(s)	Soluble in organic solvents	Budavari 1989
Partition coefficients:		
Log K _{ow}	1.32	HSDB 1992
Log K _{oc}	1.81	EPA 1982
Vapor pressure:		
at 20°C	500 mmHg	Verschuieren 1983
at 25°C	591 mmHg	Torkelson and Rowe 1981
Henry's law constant:		
at 20-25°C	0.19 atm·m ³ /mol	Pankow and Rosen 1988
Autoignition temperature	570.0°C	HSDB 1992
Flashpoint	-16°C (open-cup) -19°C (closed-cup)	EPA 1985a EPA 1985a
Flammability limits	7.3-16%	Weiss 1986
Conversion factors	1 ppm = 3.97 mg/m ³ 1 mg/m ³ = 0.25 ppm	Verschuieren 1983 Verschuieren 1983
Explosive limits	5.6-11.4% v/v in air	Sax and Lewis 1987