

## CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

Chloroethane (also known as ethyl chloride) is a colorless gas at room temperature and pressure. When stored in pressurized containers, it is a liquid. It has a characteristically sharp pungent smell (NLM 2023). Information regarding the chemical identity of chloroethane is presented in Table 4-1.

**Table 4-1. Chemical Identity of Chloroethane**

Characteristic	Information	Reference
Chemical name	Ethyl chloride; chloroethane	Lide 2005
Synonym(s) and registered trade name(s)	Aethylis; chloridum; chlorethyl; ether chloratus; ether hydrochloric; ether muriatic; ethyl chloride; monochloroethane; Anodynon; Chelen; chloryl anesthetic; Kelene; Narcotile	NLM 2023
Chemical formula	C <sub>2</sub> H <sub>5</sub> Cl	NLM 2023
SMILES	CCCl	NLM 2023
Chemical structure	CH <sub>3</sub> -CH <sub>2</sub> -Cl	NLM 2023
CAS Registry Number	75-00-3	NLM 2023

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

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Chloroethane is a colorless gas under standard atmospheric and temperature conditions. It is considered a flammable gas and should not be used in areas where ignition may occur (NLM 2023). In the environment, it is highly volatile and tends to partition to the atmosphere. Information regarding the physical and chemical properties of chloroethane is presented in Table 4-2.

**Table 4-2. Physical and Chemical Properties of Chloroethane**

Property	Information	Reference
Molecular weight	64.51 g/mol	NLM 2023
Color	Colorless	NLM 2023
Physical state	Gas	NLM 2023
Melting point	-138.7°C	Budavari et al. 1989
Boiling point	32.5°C at 2 atm; 12.3°C at 760 torr	Budavari et al. 1989, 1996

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**Table 4-2. Physical and Chemical Properties of Chloroethane**

Property	Information	Reference
Specific gravity at 0°C	0.9214	Budavari et al. 1996
Density at 20°C	0.8970	Morris and Tasto 1979
Odor	Ethereal, pungent	NLM 2023
Odor threshold:		
Water	0.019 ppm (w/v)	Amoore and Hautala 1983
Air	4.2 ppm (v/v) (11.3 g/L)	Amoore and Hautala 1983
Solubility:		
Water at 20°C	0.574 g/100 mL	Budavari et al. 1989
Organic solvents	Alcohol: 48.3 g/100 mL	Budavari et al. 1989
Partition coefficients:		
Log K <sub>ow</sub>	1.43	NLM 2023
Log K <sub>oc</sub>	1.52 (estimated using equation 4–7)	Lyman 1982
K <sub>oc</sub>	143; 33 (using log K <sub>oc</sub> of 1.52)	Lyman 1982
Vapor pressure at 20°C	1,008 mmHg	Daubert and Danner 1985
Henry's law constant at 25°C	1.11x10 <sup>-2</sup> atm•m <sup>3</sup> /mole (24.8 C)	Gossett 1987
Autoignition temperature	519°C	Morris and Tasto 1979
Flashpoint		
Open cup	-43°C	Budavari et al. 1989
Closed cup	-50°C	Budavari et al. 1989
Conversion factors:		
ppm (v/v) to mg/m <sup>3</sup> in air (20°C)	ppm (v/v) x 2.68 = mg/m <sup>3</sup>	Budavari et al. 1989
mg/m <sup>3</sup> to ppm in air (20°C)	mg/m <sup>3</sup> x 0.373 = ppm (v/v)	Budavari et al. 1989
Explosive limits in air	3.8–15.4 volume %	NLM 2023