3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of chloromethane is located in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of chloromethane is located in Table 3-2.

3. CHEMICAL AND PHYSICAL INFORMATION

Table 3-1. Chemical Identity of Chloromethane

Characteristic	Information	Reference
Chemical name	Chloromethane	CAS 1988; Weast 1988
Synonym(s)	Methyl chloride, monochloromethane	CAS 1988; SANSS 1988
Registered trade name(s)	Artic R 40 Freon 40	HSDB 1998; SANSS 1988
Chemical formula	CH_3Cl	CAS 1988
Chemical structure		EPA 1991b

$$H—C—Cl$$ with H above and H below (H bonded to central C)

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        H
        |
  H  —  C  —  Cl
        |
        H
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Identification numbers:

CAS Registry	74-87-3	CAS 1988
NIOSH RTECS	PA6300000	RTECS 1988
EPA Hazardous Waste	UO45	HSDB 1998
OHM/TADS	7216794	OHM-TADS 1988
DOT/UN/NA/IMCO Shipping	UN 1063; IMO2.0	HSDB 1998; RTECS 1988
HSDB	883	HSDB 1998
NCI	No data	

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

3. CHEMICAL AND PHYSICAL INFORMATION

Table 3-2. Physical and Chemical Properties of Chloromethane

Property	Information	Reference
Molecular weight	50.49	Weast 1988
Color	Colorless	Holbrook 1992
Physical state	Gas	Holbrook 1992; Weast 1988
Melting point	-97.7 °C	Holbrook 1992
	-97.1 °C	Weast 1988
Boiling point	-23.73 °C	Holbrook 1992
	-24.2 °C	Weast 1988

Density:
    Liquid at 20/4 °C
    Gas at 0 °C, 1 atm
	
	0.920 g/mL
	2.3045 g/L
		
		Holbrook 1992
		Holbrook 1992

Specific gravity	1.74 (air = 1)	Holbrook 1992
Odor	Ethereal, nonirritating	Merck 1989

Odor threshold:
    Water
    Air
	
	No data
	10.0 ppm (21 mg/m^3)
	21 mg/m^3 (10 ppm)
		
		Fazzalari 1978
		EPA 1991b

Solubility:
    Fresh water at 25 °C
 	
    Fresh water at 20 °C
	
	5,325 mg/L
	4,800 mg/L
	3,030 mL/L
		
		Horvath 1982
		Holbrook 1992
		Merck 1989

Organic solvents[a]
    Benzene
    Carbon tetrachloride
    Glacial acetic acid
    Absolute alcohol
	
	4,723 (99,200 mg/L)
	3,756 (78,900 mg/L)
	3,679 (77,259 mg/L)
	3,740 (78,540 mg/L)
		
		Holbrook 1992
		Holbrook 1992
		Holbrook 1992
		Holbrook 1992

Partition coefficients:
    Log K_{ow}
 	
    Log K_{oc}
	
	0.91 (experimental)
	1.086 (calculated)
	Does not tend to adsorb to soil
		
		Hansch and Leo 1985
		SRC 1995
		HSDB 1998; Lyman 1982

Vapor pressure:
    at 20 °C
    at 25 °C
	
	3,670 mmHg (489 kPa)
	4,310 mmHg (575 kPa)
		
		Holbrook 1992
		Riddick et al. 1986

Henry's law constant: at 25 °C	 8.82x10^{-3} atm-m^3/mol 8.88 x 10^{-3} atm-m^3/mol	 Gossett 1987 SRC 1994

Table 3-2. Physical and Chemical Properties of Chloromethane (continued)

Property	Information	Reference
Hydrolysis half-life	0.93 years at 25 °C 88 years at 0 °C 14 years at 10 °C 0.7–1.1 years at 25 °C 4.6 years at 15 °C 2.5 years at 20 °C ≈ 2 years at 20°C	Mabey and Mill 1978 Zafiriou 1975 Zafiriou 1975 Elliot and Rowland 1995 Elliot and Rowland 1995 Zafiriou 1975 Heppolette and Robertson 1959
Half-life resulting from reaction with hydroxyl radicals in the atmosphere	0.5 years 0.75–2 years 1–2 years 2–3 years	Crossley 1997; Atkinson 1985 Atkinson 1985 Khalil and Rasmussen 1981 Crutzen and Gidel 1983; Singh et al. 1979
Half-life resulting from photodissociation in the upper atmosphere (30 km)	2.2 years	Robbins 1976
Autoignition temperature	632 °C	Holbrook 1992
Flashpoint, open cup	-46°C	Holbrook 1992
Flammability limits	10.7–17.4 vol % 8.1–17.2 vol:vol	Holbrook 1992 Merck 1989; NFPA 1994
Reactivities	Reacts with ammonia to form methyl amine hydrochlorides; slowly decomposes in presence of water to form HCl, which is corrosive to metals	Holbrook 1992
	Reacts explosively with lithium, sodium, potassium, magnesium. Spontaneously flammable aluminum trimethyl formed upon reaction of chloromethane with aluminum in presence of trace aluminum chloride	NFPA 1994
Conversion factors: ppm (v/v) to mg/m^3 in air at 25 °C mg/m^3 to ppm (v/v) in air at 25 °C	ppm (v/v) x 2.064 = mg/m^3 mg/m^3 x 0.4845 = ppm (v/v)	Calculated

[a] Gas, 20 °C, 1 atm, mL CH$_3$Cl/100 mL solvent.