CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Industrial chloromethane is a colorless compressed gas or liquid, commonly stored and shipped as a liquified compressed gas. Chloromethane in the environment is mainly from natural sources and is a trace component of the atmosphere. Chloromethane is composed of a single carbon atom bound to three hydrogen atoms and one chlorine atom. Chloromethane was previously used as a refrigerant; however, this use has been replaced by other chemicals such as hydrofluorocarbons. Although chloromethane has a faint sweet odor, at some time after a series of chloromethane-related deaths in 1928 and 1929, acrolein was added to chloromethane refrigerants as a nasal irritating tracer to help warn those who might be exposed (McNally 1946). Chloromethane is currently used as an industrial solvent; in the production of adhesives, sealants, silicones, agricultural chemicals, plastic, and rubber products; as a chemical intermediate; in paints and coatings; and in personal care products. It is also an impurity in vinyl chloride and may be present in polyvinyl chloride (PVC) products. Chloromethane is produced from methanol and hydrogen chloride using an aluminum oxide catalyst (PubChem 2022).

Table 4-1 lists common synonyms, trade names, and other pertinent identification information for chloromethane.

Characteristic	Information
Synonym(s) and registered trade name(s)	Chloromethane; methyl chloride; methane, chloro-; monochloromethane; methylchlorid; MeCl; chloride, methyl; R 40; Artic; Freon 40; Refrigerant R40; UNII A6R43525YO; EPA (RCRA) hazardous waste number U045
Chemical formula	CH₃CI
Chemical structure	H ₃ C—CI
CAS Registry Number	74-87-3

Table 4-1. C	Chemical Identit	ty of Chloromethan
--------------	------------------	--------------------

CAS = Chemical Abstracts Service

Source: PubChem 2022

CHLOROMETHANE

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Chloromethane exists as a gas at room temperature and atmospheric pressure. It is highly soluble in water and several other organic solvents such as benzene, carbon tetrachloride, acetic acid, and ethanol. It is miscible in chloroform and ether. Chloromethane has a high vapor pressure and is extremely flammable. In addition to being highly water soluble, chloromethane has a low K_{ow} value, suggesting that it is unlikely to bioaccumulate. Chloromethane's low K_{oc} indicates a high mobility in soil. The Henry's Law constant for chloromethane suggests that it will rapidly volatilize from the surface of water and that it may volatilize from moist soil; the high vapor pressure of chloromethane indicates that it will volatilize from dry soil surfaces. Table 4-2 lists important physical and chemical properties of chloromethane.

Property	Information	Reference
Molecular weight	50.488 g/mol	Tsai 2017
Color	Colorless	PubChem 2022
Physical state	Gas (can leak as a liquid or vapor)	PubChem 2022
Melting point(s)	-97°C; -97.6°C; -97.7°C	PubChem 2022
Boiling point(s)	-23.7°C; -24.0°C	PubChem 2022
Critical temperature and pressure	416.25 K and 6.679 MPa	PubChem 2022
Density	0.911 g/cm³ at 25°C; 0.997 g/cm³ at -24°C	PubChem 2022; Tsai 2017
Viscosity	0.106 mPas (gas at 20°C)	Tsai 2017
Taste	Sweet taste	PubChem 2022
Odor	Faint sweet ethereal odor; mild odor ^a	PubChem 2022
Odor threshold:		PubChem 2022
Water	No data	
Air	21 mg/m ^{3 a}	
Solubility:		PubChem 2022
Water	5,040 mg/L at 25°C	
Organic solvent(s) at 20°C	Benzene 4,723 mg/L, carbon tetrachloride 3,756 mg/L, glacial acetic acid 3,679 mg/L, ethanol 3,740 mg/L; miscible with ethyl ether, acetone, benzene, and chloroform	
Partition coefficients:		
Log K _{oa}	1.565	Vallero 2014
Log Kow	0.91	PubChem 2022
Log K _{oc}	13 (estimated)	EPA 2012a; PubChem 2022
Relative vapor density	1.8 (air=1)	PubChem 2022; Tsai 2017

Table 4-2. Physical and Chemical Properties of Chloromethane

Table 4-2.	Physical a	and Chemical	Properties	of	Chloromethane
------------	------------	--------------	------------	----	---------------

Property	Information	Reference
Vapor pressure at 25°C	4300 mmHg	PubChem 2022
Henry's law constant at 24°C	8.82x10 ⁻³ atm-m ³ /mol	PubChem 2022
Degradation half-life in air via reaction with OH radicals	445 days (based on an OH radical rate constant of $3.6x10^{-14}$ cm ³ /molecule-second at 25°C)	PubChem 2022
Dissociation constants:	Not applicable	
Heat of combustion	-5,290 Btu/lb; -2,939 cal/g; -123.1X10 ⁺⁵ J/kg	PubChem 2022
Heat of vaporization	18.92 kJ/mol at 25°C 21.40 kJ/mol at boiling point	PubChem 2022
Autoignition temperature	632°C	PubChem 2022
Flashpoint	-50°F (closed cup); -45.6°C	PubChem 2022
Flammability limits in air	8.1% (lower explosive limit); 17.4% (upper explosive limit)	PubChem 2022; Tsai 2017
Conversion factors:	1 mg/L = 484 ppm; 1 ppm = 2.06 mg/m³ at 25°C and 760 torr	PubChem 2022
Explosive limits	Moderate explosion hazard when exposed to flames and sparks	PubChem 2022
Incompatibilities and reactivity	Chloromethane will attack some forms of plastics, rubber, and coatings; also attacks aluminum, magnesium and zinc; Incompatible with strong oxidizing agents and iron	PubChem 2022

^aChloromethane odor is not noticeable at dangerous concentrations.