# 3. CHEMICAL AND PHYSICAL INFORMATION

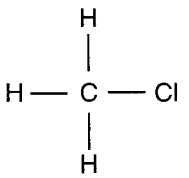
## 3.1 CHEMICAL IDENTITY

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.

## 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<br>R 40<br>Freon 40 | HSDB 1998; SANSS 1988 |
| Chemical formula | $CH_3Cl$ | CAS 1988 |
| Chemical structure |  | EPA 1991b |
| 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

## 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<br>-97.1 °C | Holbrook 1992<br>Weast 1988 |
| Boiling point | -23.73 °C<br>-24.2 °C | Holbrook 1992<br>Weast 1988 |
| Density: | | |
| Liquid at 20/4 °C | 0.920 g/mL | Holbrook 1992 |
| Gas at 0 °C, 1 atm | 2.3045 g/L | Holbrook 1992 |
| Specific gravity | 1.74 (air = 1) | Holbrook 1992 |
| Odor | Ethereal, nonirritating | Merck 1989 |
| Odor threshold: | | |
| Water | No data | |
| Air | 10.0 ppm (21 mg/m$^3$)<br>21 mg/m$^3$ (10 ppm) | Fazzalari 1978<br>EPA 1991b |
| Solubility: | | |
| Fresh water at 25 °C | 5,325 mg/L<br>4,800 mg/L | Horvath 1982<br>Holbrook 1992 |
| Fresh water at 20 °C | 3,030 mL/L | Merck 1989 |
| Organic solvents[a] | | |
| Benzene | 4,723 (99,200 mg/L) | Holbrook 1992 |
| Carbon tetrachloride | 3,756 (78,900 mg/L) | Holbrook 1992 |
| Glacial acetic acid | 3,679 (77,259 mg/L) | Holbrook 1992 |
| Absolute alcohol | 3,740 (78,540 mg/L) | Holbrook 1992 |
| Partition coefficients: | | |
| Log $K_{ow}$ | 0.91 (experimental)<br>1.086 (calculated) | Hansch and Leo 1985<br>SRC 1995 |
| Log $K_{oc}$ | Does not tend to adsorb to soil | HSDB 1998; Lyman 1982 |
| Vapor pressure: | | |
| at 20 °C | 3,670 mmHg (489 kPa) | Holbrook 1992 |
| at 25 °C | 4,310 mmHg (575 kPa) | Riddick et al. 1986 |
| Henry's law constant: | | |
| at 25 °C | 8.82x10$^{-3}$ atm-m$^3$/mol<br>8.88 x 10$^{-3}$ atm-m$^3$/mol | Gossett 1987<br>SRC 1994 |

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

| Property | Information | Reference |
|---|---|---|
| Hydrolysis half-life | 0.93 years at 25 °C<br>88 years at 0 °C<br>14 years at 10 °C<br>0.7–1.1 years at 25 °C<br>4.6 years at 15 °C<br>2.5 years at 20 °C<br>≈ 2 years at 20°C | Mabey and Mill 1978<br>Zafiriou 1975<br>Zafiriou 1975<br>Elliot and Rowland 1995<br>Elliot and Rowland 1995<br>Zafiriou 1975<br>Heppolette and Robertson 1959 |
| Half-life resulting from reaction with hydroxyl radicals in the atmosphere | 0.5 years<br>0.75–2 years<br>1–2 years<br>2–3 years | Crossley 1997; Atkinson 1985<br>Atkinson 1985<br>Khalil and Rasmussen 1981<br>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 %<br>8.1–17.2 vol:vol | Holbrook 1992<br>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:<br>ppm (v/v) to mg/m$^3$ in air at 25 °C<br>mg/m$^3$ to ppm (v/v) in air at 25 °C | ppm (v/v) x 2.064 = mg/m$^3$<br>mg/m$^3$ x 0.4845 = ppm (v/v) | Calculated |

[a] Gas, 20 °C, 1 atm, mL $CH_3Cl$/100 mL solvent.