

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

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

3.2 PHYSICAL AND CHEMICAL PROPERTIES

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

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Table 3-1. Chemical Identity of Chloroform

Characteristic	Information	Reference
Chemical name	Trichloromethane	SANSS 1990
Synonym(s)	Methenyl chloride, methane trichloride, methyl trichloride, formyl trichloride	IARC 1979
Registered trade name(s)	Freon 20, R 20, R 20 refrigerant	IARC 1979
Chemical formula	CHCl ₃	Weast 1988
Chemical structure	$ \begin{array}{c} \text{Cl} \\ \\ \text{H} - \text{C} - \text{Cl} \\ \\ \text{Cl} \end{array} $	IARC 1979
Identification numbers:		
CAS registry	67-66-3	Weast 1988
NIOSH RTECS	FS 9100000	HSDB 1996
EPA hazardous waste	UO44	HSDB 1996
OHM/TADS	7216639	HSDB 1996
DOT/UN/NA/IMCO shipping	Chloroform; UN 1888; IMO 6.1	HSDB 1996
HSDB	56	HSDB 1996
NCI	CO2686	HSDB 1996

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 Chloroform

Property	Information	Reference
Molecular weight	119.38	Deshon 1979
Color	Colorless	Hawley 1981
Physical state	Liquid	Deshon 1979
Melting point	-63.2 °C -64 °C -63.5 °C	Deshon 1979 Verschuieren 1983 Weast 1988
Boiling point	61.3 °C 62 °C 61.7 °C	Deshon 1979 Verschuieren 1983 Weast 1988
Density: at 20 °C	1.485 g/cm ³ 1.4832 g/cm ³	Hawley 1981 Weast 1988
Odor	Pleasant, ethereal, nonirritating Pleasant, sweet	Deshon 1979 NFPA 1994
Odor threshold:		
Water	2.4 ppm (w/v)	Amoore and Hautala 1983
Air	85 ppm (v/v)	Amoore and Hautala 1983
Solubility: Water at 25 °C	7.22x10 ³ mg/L 9.3x10 ³ mg/L 7.43 x 10 ³ mg/L	Banerjee et al. 1980 Verschuieren 1983 Merck 1989
Organic solvent(s)	Miscible with principal organic solvents Miscible with alcohol, benzene, ether, petroleum ether, carbon tetrachloride, carbon disulfide, oils	Deshon 1979 Merck 1989
Partition coefficients:		
Log K _{ow}	1.97	Hansch and Leo 1985, Verschuieren 1983
Log K _{oc}	1.65 2.40	Sabljić 1984 Aster 1996
Vapor pressure at 20 °C	159 mm Hg 160 mm Hg 160 mm Hg	Boublik et al. 1984 Verschuieren 1983 NFPA 1994
Henry's law constant:		
at 20 °C	3.0x10 ⁻³ atm-m ³ /mol	Nicholson et al. 1984
at 24.8 °C	3.67x10 ⁻³ atm-m ³ /mol	Gossett 1987
at 25 °C	4.06x10 ⁻³ atm-m ³ /mol	SRC 1994a

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

Property	Information	Reference
Decomposition rates	Negligible rate of hydrolysis Half-life of 80 days in air with photochemically produced hydroxyl radicals	Mabey and Mill 1978 Hampson 1980
	Residence time in air 116 days	Singh et al. 1981
Hydrolysis rate constant at 25 °C for pH>8	6.44×10^{-5} L/mol-sec	SRC 1994b
Autoignition temperature	>1,000 °C	Deshon 1979
Flashpoint	None	Deshon 1979
Flammability limits	No data	No data
Conversion factors in air (20 °C)	1 ppm (v/v)=4.96 mg/m ³	Calculated
	1 mg/m ³ =0.20 ppm (v/v)	Calculated
Other	Reacts with strong alkalies and aluminum	NFPA 1994
	<i>Oxidized by strong oxidizing agents such as chromic acid, with formation of phosgene and chlorine gas</i>	HSDB 1996
Explosive limits	No data	No data

v/v = volume per volume; w/v = weight per volume