

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Common synonyms, trade names, and other pertinent identification information for methyl mercaptan are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Important physical and chemical properties of methyl mercaptan are listed in Table 3-2.

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TABLE 3-1. Chemical Identity of Methyl Mercaptan

Characteristic	Information	Reference
Chemical name	Methyl mercaptan	Windholz 1983
Synonyms	Methanethiol; thiomethyl alcohol; methyl sulfhydrate; mercaptomethane; thiomethanol	HSDB 1989; Windholz 1983
Trade names	No data	
Chemical formula	CH ₄ S	Windholz 1983
Chemical structure	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{SH} \\ \\ \text{H} \end{array}$	
Identification numbers:		
CAS Registry	74-93-1	Sax and Lewis 1987
NIOSH RTECS	PB4375000	HSDB 1989
EPA Hazardous Waste	U153	NLM 1989
OHM/TADS	No data	
DOT/UN/NA/IMCO Shipping	UN 1064	NLM 1989
	IMCO 2.0	HSDB 1989
HSDB	813	NLM 1989
NCI	No data	

CAS - Chemical Abstracts Service; 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 Methyl Mercaptan

Property	Information	Reference
Molecular weight	48.11	Windholz 1983
Color	Colorless	Verschuieren 1983
Physical state	Gas	Verschuieren 1983
Melting point	-123.1°C	Verschuieren 1983
Boiling point	5.95°C	Windholz 1983
Density at 20°C	0.8665	Windholz 1983
Odor	Rotten cabbage	Windholz 1983
Odor threshold:		
Water	0.000024 mg/L	Amoore and Hautala 1983
Air	0.0016 ppm	Amoore and Hautala 1983
Solubility:		
Water at 20°C	23.3 g/L	Windholz 1983
Water at 25°C	15.39 g/L	Hine and Mookerjee 1975
Organic solvents	Soluble in alcohol, ether, petroleum, naphtha	Sax and Lewis 1987
Partition coefficients:		
Log K_{ow}	No data	
Log K_{oc}	No data	
Vapor Pressure at 25°C	1,500 mmHg	EPA 1983
pKa	No data	
Henry's law constant	3.85×10^{-3} atm-m ³ /mol	EPA 1983
Autoignition temperature	No data	
Flashpoint	0°F (-18°C) (open cup)	HSDB 1989
Flammability limits	No data	
Conversion factors	1 ppm = 2.05 mg/m ³ 1 mg/m ³ = 0.488 ppm	Verschuieren 1983
Explosive limits	3.9%-21.8%	Sax and Lewis 1987