

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Methyl *tert*-butyl ether (MTBE) is a volatile organic compound (VOC) often added to gasoline to reduce air pollution. MTBE and other components, commonly known as “oxygenates,” are added to gasoline to increase the octane number and reduce carbon monoxide emissions. Information regarding the chemical identity of MTBE is located in Table 3- 1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

MTBE is a relatively volatile chemical and is moderately soluble in water. It is very soluble in some organic solvents such as alcohol and ether. Oil refiners blend MTBE into gasoline to meet requirements for oxygenated fuels. Gasoline containing MTBE has become recognizable by its pungent odor. MTBE is flammable, and is a moderate fire risk (Sax and Lewis 1987). Information regarding the physical and chemical properties of MTBE is located in Table 3-2.

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Table 3-1. Chemical Identity of Methyl *tert*-Butyl Ether (MTBE)

Characteristic	Information	Reference
Chemical Name	Methyl <i>tert</i> -butyl ether	Merck 1989
Synonyms	<i>tert</i> -Butyl methyl ether; 2-methoxy-2-methylpropane; MTBE; methyl <i>t</i> -butyl ether;	Merck 1989
Registered trade names	No data	
Chemical formula	C ₅ H ₁₂ O	Merck 1989
Chemical structure	$ \begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{O} - \text{CH}_3 \\ \\ \text{CH}_3 \end{array} $	
Identification numbers:		
CAS Registry	1634-04-4	Merck 1989
NIOSH RTECS	KCN5250000	HSDB 1995
EPA Hazardous Waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO Shipping	UN 2398; IMO 3.2	HSDB 1995
HSBD	5847	HSDB 1995
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. Chemical and Physical Properties of Methyl *tert*-Butyl Ether (MTBE)

Property	Information	Reference
Molecular weight	88.15	Lide 1994
Color	Colorless	HSDB 1994
Physical state	Liquid	Merck 1989
Melting point	-109 °C	Lide 1994
Boiling point	55.2 °C	Lide 1994
Density at 20 °C	0.7405 g/cc	Lide 1994
Odor at 25 °C	terpene-like	Gilbert and Calabrese 1992
Odor threshold, in water	680 ppb	Gilbert and Calabrese 1992
Solubility:		
Water	4.8 g/100 g water	Merck 1989
Water, 20 °C	4–5%	Gilbert and Calabrese 1992
Organics	soluble in alcohol, ether	Lide 1994
Partition coefficients:		
Log K _{ow}	1.24	
Log K _{oc}	1.05 (estimated) 2.89 (calculated)	Gilbert and Calabrese 1992 EPA 1995
Vapor pressure at 25 °C	245 mm Hg	Merck 1989
Henry's law constant at 25 °C	5.87×10^{-4} atm-m ³ /mol	Hine and Mookerjee 1975
Ignition temperature	224 °C	Merck 1989
Flashpoint	-28 °C	Merck 1989
	28 °C (closed cup)	Gilbert and Calabrese 1992
Flammability limits	No data	
Conversion factors		
ppm (v/v) to mg/m ³ in air at 25 °C	1 ppm = 3.61 mg/m ³	
mg/m ³ to ppm (v/v) in air at 25 °C	1 mg/m ³ = 0.28 ppm	
Explosion limits	1.65 to 8.4% in air	Gilbert and Calabrese 1992
Other	MTBE is unstable in acidic solution	Merck 1989

