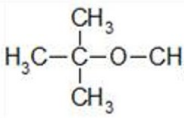
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

MTBE is a VOC that was added to gasoline to reduce air pollution. MTBE and other components, commonly known as "oxygenates," were added to gasoline to increase the octane number and reduce carbon monoxide emissions. Information regarding the chemical identity of MTBE is presented in Table 4-1.

Table 4-1. Chemical Identity of Methyl *tert*-Butyl Ether (MTBE)

Characteristic	Information	Reference
Chemical name	Methyl *tert*-butyl ether	Budavari 1989
Synonym(s) and registered trade name(s)	*tert*-Butyl methyl ether; 2-methoxy-2-methylpropane; MTBE; methyl *t*-butyl ether	Budavari 1989
Chemical formula	$C_5H_{12}O$	Budavari 1989
Chemical structure		
CAS Registry Number	1634-04-4	Budavari 1989

CAS = Chemical Abstracts Service

4.2 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. MTBE is flammable and is a moderate fire risk (Lewis 1987). Information regarding the physical and chemical properties of MTBE is presented in Table 4-2.

Table 4-2. Physical and Chemical Properties of Methyl *tert*-Butyl Ether (MTBE)

Property	Information	Reference
Molecular weight	88.15	Lide 1994
Color	Colorless	Winterberg et al. 2012
Physical state	Liquid	Budavari 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	Terpene-like	Gilbert and Calabrese 1992
Odor threshold:		
Water	15–680 ppb	Angle 1991; EPA 1997; Gilbert and Calabrese 1992
Air	180 ppb	Prah et al. 1994
Solubility:		
Water at 20°C	4–5%	Gilbert and Calabrese 1992
Organic solvents	Soluble in alcohol, ether	Lide 1994
Partition coefficients:		
Log K_{ow}	0.94	NLM 2020
Log K_{oc}	1.05 (estimated) 2.13±0.060 (measured)	Gilbert and Calabrese 1992 Greenwood et al. 2007
Vapor pressure at 20°C	245 mm Hg at 25°C	Budavari 1989
Henry's law constant at 25°C	5.87×10^{-4} atm-m^3/mol	Hine and Mookerjee 1975
Autoignition temperature	224°C	Budavari 1989
Flashpoint	-28°C	Budavari 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	
Explosive limits	1.65–8.4% in air	Gilbert and Calabrese 1992