

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

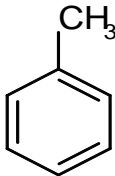
Information regarding the chemical identity of toluene is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of toluene is located in Table 4-2.

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Table 4-1. Chemical Identity of Toluene

Characteristic	Information	Reference
Chemical name	Toluene	HSDB 2010
Synonym(s)	Methylbenzene; phenylmethane; benzene, methyl-; toluol; methylbenzol	Haynes et al. 2013; HSDB 2010
Registered trade name(s)	Methacide; Antisal 1A	HSDB 2010
Chemical formula	C ₇ H ₈	Haynes et al. 2013; HSDB 2010
Chemical structure		Haynes et al. 2013; HSDB 2010
Identification numbers:		
CAS registry	108-88-3	Haynes et al. 2013
NIOSH RTECS	XS5250000	RTECS 2014
EPA hazardous waste	U220	HSDB 2010
OHM/TADS	7216928	NFPA 1994
DOT/UN/NA/IMCO shipping	UN 1294	HSDB 2010
IMCO	3.2	HSDB 2010
HSDB	131	HSDB 2010
NCI	CO7272	HSDB 2010

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; NFPA = National Fire Protection Association; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

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Table 4-2. Physical and Chemical Properties of Toluene

Property	Information	Reference
Molecular weight	92.13	Fabri et al. 2012
Color	Colorless	Haynes et al. 2013
Physical state	Liquid	Haynes et al. 2013
Melting point	-94.991°C	Fabri et al. 2012
Boiling point	110.625°C	Fabri et al. 2012
Density: at 20°C	0.8631 g/cm ³	Fabri et al. 2012
Vapor density	3.1 (air=1)	HSDB 2010
Odor	Sweet, pungent, benzene-like odor	HSDB 2010
Odor threshold:		
Water	0.024–0.17 mg/L	WHO 2004
Air	2.14 ppm (8 mg/m ³)	HSDB 2010
Solubility:		
Water at 25°C	526 mg/L	HSDB 2010
Organic solvent(s)	Miscible with alcohol, chloroform, ether, acetone, glacial acetic acid, and carbon disulfide	HSDB 2010
Partition coefficients:		
Log K _{ow}	2.73	HSDB 2010
Log K _{oc}	1.57–2.25	HSDB 2010
Vapor pressure at 25°C	28.4 mm Hg	HSDB 2010
Henry's law constant:	6.64x10 ⁻³ atm-m ³ /mol	HSDB 2010
Autoignition temperature	480°C (896°F)	HSDB 2010
Flashpoint	4°C (40°F, closed cup); 16°C (open cup)	HSDB 2010
Flammability limits	1.1–7.1%	HSDB 2010
Conversion factors ppm (v/v) to mg/m ³ in air (20°C)	1 ppm=3.76 mg/m ³	HSDB 2010
Explosive limits	1.27% lower limit	Fabri et al. 2012; HSDB 2010

v/v = volume for volume