

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

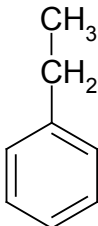
Ethylbenzene is an aromatic hydrocarbon that occurs naturally in petroleum and is a component of aviation and automotive fuels. It is used as a solvent and in the production of synthetic rubber and styrene. Information regarding the chemical identity of ethylbenzene is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Ethylbenzene is a colorless liquid with an aromatic odor. Information regarding the physical and chemical properties of ethylbenzene is located in Table 4-2. Ethylbenzene is a flammable and combustible liquid. Vapors are heavier than air and may travel to a source of ignition and flash back. Liquid ethylbenzene floats on water and may travel to a source of ignition and spread fire. Combustion may produce irritants and toxic gases (HSDB 2009; NFPA 1994). Ethylbenzene may accumulate static electricity and will react with oxidizing materials (HSDB 2009; NFPA 1994).

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Table 4-1. Chemical Identity of Ethylbenzene

Characteristic	Information	Reference
Chemical name	Ethylbenzene	Budavari and O'Neil 1989
Synonym(s)	EB; ethyl benzene; benzene, ethyl-; ethylbenzol; phenylethane; etilbenzene; ethylbenzeen; aethylbenzo; etylobenzen	HSDB 2009
Registered trade name(s)	No data	
Chemical formula	C ₈ H ₁₀	Cannella 2007
Chemical structure		Cannella 2007
Identification numbers:		
CAS registry	100-41-4	Cannella 2007
NIOSH RTECS	NIOSH/DA0700000	NIOSH 2009; RTECS 2009
EPA hazardous waste	F003	HSDB 2009
OHM/TADS	7216709	HSDB 1995
DOT/UN/NA/IMDG shipping	UN 1175; IMDG 3.2	HSDB 2009
HSDB	84	HSDB 2009
NCI	NCI-C56393	HSDB 2009
STCC	49 091 63	HSDB 2009

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = 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; STCC = Standard Transport Commodity Code

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Table 4-2. Physical and Chemical Properties of Ethylbenzene

Property	Information	Reference
Molecular weight	106.17	Lide 1994
Color	Colorless	Welch et al. 2005
Physical state	Liquid	Welch et al. 2005
Melting point	-94.975 °C	Cannella 2007
Boiling point	136.19 °C	Cannella 2007
Density at 20 °C/4 °C	0.8670	Welch et al. 2005
at 25 °C/25 °C	0.8671	Cannella 2007
Odor	Sweet, gasoline-like	CHRIS 1985
Odor threshold:		
Water	0.029 mg/L	Amoore and Hautala 1983
	0.140 mg/L	Rosen et al. 1963; Verschueren 1983
Air	2.3 ppm	Amoore and Hautala 1983
	2–2.6 mg/m ³	Verschueren 1983
Solubility:		
Water at 0 °C	197 mg/L	Polak and Lu 1973
at 15 °C	140 mg/L	Verschueren 1983
at 20 °C	152 mg/L	Verschueren 1983
at 25 °C	160 mg/L	Amoore and Hautala 1983
at 25 °C	177 mg/L	Polak and Lu 1973
at 25 °C	208 mg/L	Bohon and Claussen 1951
Organic solvents	Miscible with usual organic solvents	Budavari and O'Neil 1989
	Soluble in alcohol and ether	Lide 1994
Partition coefficients:		
Log K _{ow}	4.34	EPA 1982
	3.13	Yalkowsky and Valvani 1976
	3.15	Hansch et al. 1995
Log K _{oc}	2.22 (calculated)	Chiou et al. 1983
	2.38 (measured)	Hodson and Williams 1988
	2.40 (calculated)	Vowles and Mantoura 1987
Vapor pressure		
at 20 °C	7 mm Hg	Verschueren 1983
at 25 °C	1.27 kPa (9.53 mm Hg)	Mackay and Shiu 1981
at 25.9 °C	10 mm Hg	Sax and Lewis 1989
at 30 °C	12 mm Hg	Verschueren 1983

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Table 4-2. Physical and Chemical Properties of Ethylbenzene

Property	Information	Reference
Henry's law constant:		
at 20 °C	6.6×10^{-3} atm-m ³ /mol	EPA 1982
at 20 °C	8.7×10^{-3} atm-m ³ /mol	Lyman et al. 1982
at 25 °C	8.43×10^{-3} atm-m ³ /mol	Mackay et al. 1979
at 25 °C	7.9×10^{-3} atm-m ³ /mol	Mackay and Shiu 1981
Autoignition temperature	810 °F (432 °C)	Cannella 2007; NFPA 1994;
Flash point	15 °C	Cannella 2007
Flammability limits	0.8 (lower) vol% –6.7 (upper) vol%	NIOSH 2005
Conversion factors (25 °C, 1 atm)	1 mg/m ³ =0.230 ppm 1 ppm=4.34 mg/m ³	NIOSH 2005; Verschueren 1983