4. CHEMICAL AND PHYSICAL INFORMATION

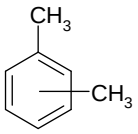
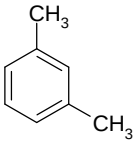
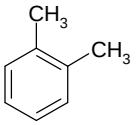
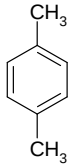
4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of *m*-, *o*-, and *p*-xylene and mixed xylene is located in Table 4-1. Commercial or mixed xylene generally contains about 40–65% *m*-xylene and up to 20% each of *o*-xylene, *p*-xylene, and ethylbenzene (Fishbein 1985).

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of *m*-, *o*-, and *p*-xylene and mixed xylene is located in Table 4-2.

Table 4-1. Chemical Identity of *m*-Xylene, *o*-Xylene, *p*-Xylene, and Mixed Xylene[a]

Characteristics	Mixed xylene	*m*-Xylene	*o*-Xylene	*p*-Xylene
Synonyms/trade names	Dimethylbenzene; xylol; benzene, dimethyl-; ksylen (Polish); xiloli (Italian); xylenen (Dutch); xylole (German); methyl toluene[b]; Violet 3[b]	1,3-Dimethyl-benzene[c]; benzene, 1-3-dimethyl-; *m*-di-methylbenzene; *m*-methyltoluene; 1,3-xylene; *m*-xylol[c]; *meta*-xylene[c]	1,2-Dimethyl-benzene[c]; benzene, 1,2-dimethyl-; *o*-di-methylbenzene; *o*-methyltoluene[b]; 1,2-xylene; *o*-xylol[c]; *ortho*-xylene[c]	1,4-Dimethyl-benzene[c]; benzene, 1,4-di-methyl-; *p*-di-methylbenzene; *p*-methyltoluene; 1,4-xylene; *p*-xylol[c]; *para*-xylene[c]
Chemical formula	C_8H_{10}	C_8H_{10}	C_8H_{10}	C_8H_{10}
Chemical structure				
Identification numbers:				
CAS registry	1330-20-7	108-38-3	95-47-6	106-42-3
NIOSH RTECS	ZE2100000[d]	ZE2275000[d]	ZE2450000[d]	ZE2625000[d]
EPA hazardous waste	U239; F003	U239; F003	U239; F003	U239; F003
DOT/UN/NA/IMCO shipping	UN 1307; IMCO3.2; IMCO3.3	UN 1307; IMCO3.2; IMCO3.3	UN 1307; IMCO3.2; IMCO3.3	UN 1307; IMCO3.2; IMCO3.3
HSDB	4500	135	134	136
NCI	C55232	No data	No data	No data
STCC	49 093 50	49 093 50	49 093 50	49 093 51

[a]All information obtained from HSDB 2007 except where noted.
[b]Lewis 2000
[c]NIOSH 2005
[d]RTECS 2007

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/Intergovernmental 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; RTECS = Registry of Toxic Effects of Chemical Substances; STCC = Standard Transport Commodity Code

Table 4-2. Physical and Chemical Properties of *m*-Xylene, *o*-Xylene, *p*-Xylene, and Mixed Xylene[a]

Property	Mixed xylene	*m*-Xylene	*o*-Xylene	*p*-Xylene
Molecular weight	106.16[b]	106.16[b]	106.16[b]	106.16[b]
Color	Clear[c]	Colorless[c]	Colorless[c]	Colorless[c]
Physical state	Liquid[c]	Liquid[c]	Liquid[c]	Liquid[c]
Melting point	No data	-47.8 °C[d]	-25.2 °C[d]	13.2 °C[d]
Boiling point	137–140 °C[b]	139.1 °C[d]	144.5 °C[d]	138.4 °C[d]
Density at 20 °C/4 °C	0.864 g/cm^3[e]	0.864 g/cm^3[e]	0.880 g/cm^3[e]	0.8611 g/cm^3[e]
Odor	Sweet	Sweet	Sweet	Sweet
Odor threshold:				
Water	No data	No data	No data	No data
Air	0.0045 mg/L (1.0 ppm)[g]	0.05 ppm[f]	0.05 ppm[f]	0.05 ppm[f]
Solubility:				
Water at 25 °C	106 mg/L[i]	161 mg/L[j]	178 mg/L[j]	162 mg/L[j]
Organic solvent(s)	Miscible with alcohol and ether[b]	Miscible with alcohol, ether, and other solvents[b]	Miscible with alcohol and ether[b]	Soluble in alcohol, ether, and other organic solvents[b]
Partition coefficients:				
Log K_{ow}	No data	3.2[k]	3.12[k]	3.15[k]
Log K_{oc}	No data	2.22[l]	2.11[l]	2.31[l]
Vapor pressure	6.72 mmHg at 21°C [e]	8.29 mmHg at 25 °C[m]	6.61 mmHg at 25 °C[n]	8.84 mm Hg at 25 °C[m]
Henry's law constant	No data	7.18x10^{-3} atm-m^3/mol[j]	5.18x10^{-3} atm-m^3/mol[j]	6.90x10^{-3} atm-m^3/mol[o]
Autoignition temperature	464 °C (867 °F)	527 °C	463 °C	528 °C
Flashpoint	29 °C (CC)[b]	27 °C (CC)[b]	32 °C (CC)[b]	27 °C (CC)[b]
Flammability limits	No data	1.1–7.0%	1.0–7.0%	1.1–7.0%
NFPA Flammability Classification	3[p]	3[p]	3[p]	3[p]
NFPA Reactivity Classification	0[q]	0[q]	0[q]	0[q]

Table 4-2. Physical and Chemical Properties of *m*-Xylene, *o*-Xylene, *p*-Xylene, and Mixed Xylene[a]

Property	Mixed xylene	*m*-Xylene	*o*-Xylene	*p*-Xylene
Air conversion factors[r]	1 ppm = 4.34 mg/m^{3}[l]	1 ppm = 4.34 mg/m^{3}[s]; 1 ppm = 4.41 mg/m^{3}[t]; 1 mg/m^{3} = 0.23ppm[s]	1 ppm = 4.34 mg/m^{3}[l]; 1 ppm = 4.41 mg/m^{3}[t]; 1 mg/m^{3} = 0.23 ppm[t]	1 ppm = 4.34 mg/m^{3}[l]; 1 ppm = 4.41 mg/m^{3}[t]; 1 mg/m^{3} = 0.23 ppm[t]

[a]All information obtained from HSDB 2007 unless otherwise noted.
[b]O'Neil et al. 2001
[c]Lewis 1997
[d]Lide 2005
[e]Lewis 2001
[f]CHRIS 1999
[g]Carpenter et al. 1975a
[h]Gerarde 1959
[i]Yalkowsky and He 1992
[j]Sanemasa et al. 1982
[k]Hansch et al. 1995
[l]Abdul et al. 1987
[m]Chao et al. 1983
[n]AIChE 1996
[o]Foster et al. 1994
[p]Classified by the NFPA as a liquid that can be ignited under almost all normal temperature conditions.
[q]Classified by the NFPA as a liquid that is normally stable even under fire exposure conditions and that is not reactive with water.
[r]In air, ppb is a volume-to-volume ratio for vapor-phase compounds like xylenes. When air monitoring data are reported in terms of ppb or ppm, it is understood that this is equivalent to ppbv or ppmv (parts per billion or parts per million volume-to-volume ratio).
[s]Sandmeyer 1981
[t]Verschueren 2001

CC = closed cup; NFPA = National Fire Protection Association; TOC = tag open cup