Appendix A

Identity, physical, chemical properties and toxicity of BTEX compounds are shown in Tables A1 to A8.

Table A1 Identity of Benzene [4]

Chemical formula	C_6H_6
CAS number	71-43-2
RTECS number	CY 1400O0
Common name	Benzene
IUPAC name	Benzene
Common synonyms	Annulene, benzine, benzol, benzole, benzol coal naphtha, cyclohexatriene, minaral naphtha, motor benzol, phenyl hydride, pyrobenzol, pyrobenzole
Purity	Nitration grade > 99%. Benzol 90 contains 80-85% benzene, 13-15% toluene and 2-3% xylene. Commercial grades are free of H_2S and SO_2 and have a maximum of 0.15% non-aromatics compounds.

Table A2 Physical and Chemical properties of Benzene [4]

Physical from (20 °C)	clear colourless liquid
Relative molecular mass	78.11
Flash point	-11.1 °C
Flammable limits	1.3-7.1%
Melting/freezing point	5.5 °C
Boiling point	80.1 °C at 760 mmHg
Density	0.878
Relative vapour density (air =1)	2.7
Vapour pressur (26 °C)	13.3 kPa
Solubilities :	
Water	1800 mg/L at 25 °C
non-aqueous solvents	miscible with most
Odour threshold	4.8-15.0 mg/m^3
Taste theshold (water)	0.5-4.5 mg/L
Log *n*-octanol/water partition coefficient	1.56-2.15
Sorption coefficient (log K_{oc}-distribution coefficient between benzene adsorbed to soil organic carbon benzene in solution)	1.8-1.9

Table A3 Identity of Toluene [5]

Chemical formula	C_7H_8
Relative molular mass	92.13
CAS chemical name	phenylmethane
CAS number	108-88-3
RTECS number	XS 5250000
Common name	methybenzene
Common trade names	methacide, methybenzol, toluol

The purification of toluene products may include azeotropic distillation with paraffinic hydrocarbons, napthenic hydrocarbons, or alcohols. Because of the variety of methods used to produce toluene, the range of impurities varies widely. Benzene is an important common impurity in technical grade of toluene. Highly-purified toluene (reagent grade and nitration grade) contains less than 0.01% benzene, while industrial grade and 90/120 grade toluene contain a significant quality of benzene. The 90/120 grade contains as much as 25%.

Table A4 Physical and Chemical properties of Toluene [5]

Flash point	4.4 °C
Flammable limits	1.17-7.10%
Melting point	-95 °C
Boiling point	110.6 °C at 760 mmHg
Density	0.8669
Specific gravity	0.8623 at 20 °C
Relative vapour density (air=1)	3.20
Vapour pressure (25 °C)	28.7 mm Hg
Percent in saturated air	3.94 (760 mm , 26 °C)
Density of saturated air-vapour mixture	1.09 (760 mm ; air =1)
Solubilities :	
Water	535 mg/L at 25 °C
Sea water	380 mg/L at 25 °C
Saturation in air	112 g/m^3 (25 °C)
Log partition coefficient (octanol/water)	2.69
Surface tension	28.53 dynes/cm (20 °C)
Liquid viscosity	0.6 cp (20 °C)
Reference index	1.4969 (20 °C)

Table A5 Identity of Ethylbenzene [6]

Chemical formula	C_8H_{10}
Relative molecular mass	106.16
Chemical name	ethylbenzene
CAS number	100-41-4
RTECS number	DA 07000000
EEC number	601-023-00-4
Synonyms	phenylethane, EB, ethylbenzol

Table A6 Physical and Chemical properties of Ethylbenzene [6]

Physical state (20 °C; 101.3 kPa)	liquid
Flash point	12 °C
	12.8
	15
Melting point	-94.95 °C
Boiling point	136.2 °C (101.3 kPa)
Density (25 °C; g/cm^3)	0.866
Vapour pressure (25 °C)	1.24 kPa at 20 °C
Refractive index (15 °C D line)	1.49857
Log partition coefficient (octanol/water)	3.13
Saturated % in air (20 °C; 101.3 kPa)	1.2
Henry's Law constant (Pa m^3/mol)	887
Log sorption partition coefficient (log K_{oc})	1.98-3.04
Water solubility (20 °C; 101.3 kPa; mg/L)	152
Explosive limits (20 °C; 101.3 kPa)	1-7.8

Table A7 Identity of Xylenes [7]

Chemical formula	C_8H_{10}	C_8H_{10}	C_8H_{10}
Chemical name	ortho-xylene	meta-xylene	para-xylene
Synonyms	1,2-dimethylbenzene o-methyltoluene 1,2- xylene o-xylol	1,3-dimethylbenzene m-methylbenzene 1,3-xylene m-xylol	1,4-dimethylbenzene p-methytoluene 1,4-xylene p-xylol
Relative molecule mass	106.16	106.16	106.16
CAS number	95-47-6	108-38-3	106-42-3
RTECS number	ZE 2450000	ZE 2275000	ZE 2625000
CAS number (mixed xylenes) ;	1330-20-7		
RTECS number (mixed xylenes) ;	ZE 210000		

Table A8 Physical and chemical properties of Xylenes [7]

	o-Xylene	m-Xylene	p-Xylene
Physical state (20 °C; 101.3 kPa)	liquid	liquid	liquid
Colour	colourless	colourless	colourless
Boiling point (°C; 101.3 kPa)	144.4	139.1	138.3
Melting point (°C; 101.3 kPa)	-25.2	-47.9	13.3
Relative density (24 °/4 °C)	0.876	0.860	0.857
Vapour prssure (kPa at 20 °C)	0.66	0.79	0.86
Flash point (°C)	30	25	25
Saturation % in air (101.3 kPa)	1.03 (32 °C)	1.03 (28 °C)	1.03 (27 °C)
Explosion limits (vol-% in air)	1.0-6	1.1-7	1.1-9
Autoignition temp (°C)	465	525	525
Octanol/water partition coefficient (log P)	3.12	3.2	3.15
Solubility in water (mg/L)	142	146	185

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