Supplementary Material (ESI) for Journal of Environmental Monitoring

SUPPLEMENTARY INFORMATION

(Jia et al., "Development and Comparison…")

Chemical properties of the 94 target compounds and 2 internal standard compounds (highlighted). MW = molecular weight; BP = boiling point; RT = retention time; TI = target ion; QI = qualifier ion. Sources: refs [i] and [ii].

Compound	CAS No.	BP (°C)	RT (min)	TI (m/z)	QI (m/z)	Compound	CAS No.	BP (°C)	RT (min)	TI (m/z)	QI (m/z)
Fluorobenzene	462-06-6	84.7	7.91	96	70	p-Xylene	106-42-3	138.4	16.42	91	106
1,3-Butadiene	106-99-0	-4.4	1.70	54	39,37	m-Xylene	108-38-3	139.1	16.42	91	106
1,2-Dichloroethylene (trans,E)	156-60-5	47.7	4.81	61	96	Bromoform	75-25-2	149.2	16.93	173	252
Methyl t-butyl ether	1634-04-4	55.2	5.18	73	57	Styrene	100-42-5	145.2	17.26	104	78
1,1-Dichloroethane	75-34-3	57.3	5.18	63	83	o-Xylene	95-47-6	144.4	17.31	91	106
Propanenitrile	107-12-0	97.4	5.50	54	55	n-Nonane	111-84-2	150.8	17.78	43	41
1,2-Dichloroethylene (Cis, Z)	156-59-2	60.5	5.98	61	96	1,1,2,2-Tetrachloroethane	79-34-5	145.1	18.21	83	131, 168
2-Butanone	78-93-3	79.6	6.03	43	72, 57	1,2,3-Trichloropropane	96-18-4	156.9	18.45	75	110
2,2-Dichloropropane	594-20-7	69.3	6.13	77	97, 41	Isopropylbenzene	98-82-8	152.4	18.57	105	120
Bromochloromethane	74-97-5	68.1	6.20	49	130	Bromobenzene	108-86-1	156.1	18.67	77	156
Chloroform	67-66-3	61.2	6.27	83	47	1,4-Dichlor-2-butene (trans, E)	110-57-6	156.1	18.85	75	89, 124
Methyl acrylate	96-33-3	80.2	6.42	55	85,27	α-Pinene	7785-70-8	155.0	18.87	93	77, 105
Ethyl acetate	141-78-6	77.1	6.53	43	45	2-Chlorotoluene	95-49-8	159.2	19.48	91	126
Tetrahydrofuran	109-99-9	64.9	6.73	42	72	n-Propylbenzene	103-65-1	159.2	19.64	91	120
1,1,1-Trichloroethane	71-55-6	74.1	6.94	97	61, 117	4-Chlorotoluene	106-43-4	162.5	19.70	91	126
Cyclohexane	110-82-7	80.7	7.29	56	84	4-ethyl toluene	622-96-8	162.0	19.98	105	120
1,2-Dichloroethane	107-06-2	83.4	7.11	62	49, 98	1,3,5-Trimethylbenzene	108-67-8	164.7	20.16	105	120
Butyl chloride	109-69-3	78.4	7.14	56	41,27	Pentachloroethane	76-01-7	159.9	20.35	167	117
1,1-Dichloropropene	563-58-6	76.5	7.25	75	110	2-ethyl toluene	611-14-3	165.2	20.55	105	120
Benzene	71-43-2	80.1	7.35	78	50	Phenol	108-95-2	181.8	21.04	94	66
Carbontetrachloride	56-23-5	76.6	7.36	117	82	tert-Butylbenzene	98-06-6	169.2	21.01	119	91, 134
Chloroacetonitrile	107-14-2	124.0	8.51	75	48	1,2,4-Trimethylbenzene	95-63-6	169.4	21.02	105	120
1,2-Dichloropropane	78-87-5	96.4	8.76	63	76, 41	n-Decane	124-18-5	174.2	21.36	57	43
Trichloroethylene	79-01-6	87.0	8.77	130	95	1,3-Dichlorobenzene	541-73-1	173.1	21.61	146	111, 75
n-Heptane	142-82-5	98.4	8.90	43	71	1,4-Dichlorobenzene	106-46-7	174.1	21.37	146	111, 75
Dibromomethane	74-95-3	97.0	8.83	174	93	sec-Butylbenzene	135-98-8	173.3	21.62	105	134
2-Nitropropane	79-46-9	120.3	9.15	43	41,27	1,2,3-trimethyl benzene	526-73-8	176.1	21.98	105	120
Bromodichloromethane	75-27-4	90.0	9.10	83	129	p-Isopropyltoluene	99-87-6	177.1	22.11	119	134
2,5-Dimethyl furan	625-86-5	93.0	9.32	96	43	d-Limonene	5989-27-5	176.5	22.24	68	93, 136
Methyl cyclohexane	108-87-2	100.9	9.69	83	55	1,2-Dichlorobenzene	95-50-1	180.4	22.35	146	111,75
Methyl methacrylate	80-62-6	100.3	9.80	41	69, 100	n-Butylbenzene	104-51-8	183.3	23.15	91	134
1,1-Dichloro-2-propanone	513-88-2	120.0	10.51	43	83	o-Cresol	95-48-7	191.0	23.24	108	79,90
1,3-Dichloropropene (Cis, Z)	10061-01-5	104.0	10.88	75	110	Hexachloroethane	67-72-1	186.9	23.58	166	201, 117
Methyl isobutyl ketone	108-10-1	116.5	11.14	43	58, 85	p-Cresol	106-44-5	202.0	23.96	107	77
Toluene	108-88-3	110.6	11.93	91	92	m-Cresol	108-39-4	202.3	23.96	107	77
1,3-Dichloropropene (Trans, E)	10061-02-6	112.0	12.16	75	110, 49	1,2-Dibromo-3-chloropropane	96-12-8	196.0	23.97	157	75
1,1,2-Trichloroethane	79-00-5	113.9	12.33	97	83, 61	Nitrobenzene	98-95-3	210.8	24.11	123	77,51
1,3-Dichloropropane	142-28-9	120.4	12.94	76	41	n-Undecane	1120-21-4	195.9	24.61	57	43
p-Bromofluorobenzene	460-00-4	152.0	18.52	174	95	1,2,4-Trichlorobenzene	120-82-1	213.0	26.84	180	145, 109
Dibromochloromethane	124-48-1	119.5	13.21	129	127	Naphthalene	91-20-3	218.0	27.01	128	102
Ethyl methacrylate	97-63-2	117.0	13.34	69	99	n-Dodecane	112-40-3	216.3	27.60	57	43
2-Hexanone	591-78-6	127.7	13.42	43	58, 71,	1,2,3-Trichlorobenzene	87-61-6	218.6	27.88	180	145
n-Octane	111-65-9	125.7	13.66	43	85	Hexachlorobutadiene	87-68-3	215.0	28.05	225	260, 190
1,2-Dibromoethane	106-93-4	131.4	13.65	107	109, 27	n-Tridecane	629-50-5	235.5	30.44	57	43
Tetrachloroethene	127-18-4	121.3	13.80	166	129	n-Tetradecane	629-59-4	253.6	32.78	57	43
Chlorobenzene	108-90-7	131.7	15.40	112	77	n-Pentadecane	629-62-9	270.7	34.21	57	43
1,1,1,2-Tetrachloroethane	630-20-6	130.5	15.64	131	117, 95	n-Hexadecane	544-76-3	286.9	35.30	57	43
Ethylbenzene	100-41-4	136.2	16.09	91	106	n-Heptadecane	629-78-7	302.2	36.22	57	43

[i] C. L. Yaws, *Chemical Properties Handbook* [electronic resource]: *physical, thermodynamic, environmental, transport, safety, and health related properties for organic and inorganic chemicals*, McGraw-Hill, New York, 2003.

[ii] D. R. Lide, *CRC Handbook of Chemistry and Physics*, CRC Press, Boca Raton, FL, 2005.