


## Supplemental data:


An approach toward quantification of organic compounds in complex environmental samples using high-resolution electrospray ionization mass spectrometry

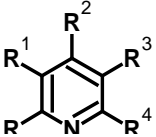
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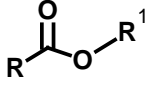
**Table S1:** Compounds used for statistical analysis in manuscript and their accompanying physical properties. Compounds are sorted by molecular mass. Data were taken from Ref <sup>1</sup> and references therein.

Heterocyclic Nitrogen (Imidazoles)		Mass (Da)	H/C	Adj. mass (Da)	PA (kJ/mol)	GB (kJ/mol)	Molecular Volume (Å <sup>3</sup> )
Imidazole		68	1.33	91	942.8	909.2	5.9
2-Methyl-1H-imidazole		82	1.50	123	963.4	929.6	7.4
4-Methyl-1H-imidazole		82	1.50	123	952.8	920.9	7.4
1,4-Dimethyl-1H-imidazole		96	1.60	154	976.7	944.9	9.0
1,2-Dimethyl-1H-imidazole		96	1.60	154	984.7	952.6	9.0
1,5-Dimethyl-1H-imidazole		96	1.60	154	977.6	945.8	9.0
1H-Benzimidazole		118	0.86	101	953.8	920.5	11.7
1-Methyl-1H-benzimidazole		132	1.00	132	967.0	935.2	13.3

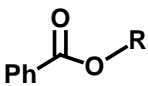
  

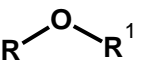
Heterocyclic Nitrogen (Pyrazoles)		Mass (Da)	H/C	Adj. mass (Da)	PA (kJ/mol)	GB (kJ/mol)	Molecular Volume (Å <sup>3</sup> )
1H-Pyrazole		68	1.33	91	894.1	860.5	5.9
1-Methyl-1H-pyrazole		82	1.50	123	912.0	880.1	7.4
3-Methyl-1H-pyrazole		82	1.50	123	906.0	874.2	7.4
4-Methyl-1H-pyrazole		82	1.50	123	906.8	873.4	7.4
1,3-Dimethyl-1H-pyrazole		96	1.60	154	933.9	902.3	9.0
1,5-Dimethyl-1H-pyrazole		96	1.60	154	934.3	902.8	9.0
3,4-Dimethyl-1H-pyrazole		96	1.60	154	927.3	895.4	9.0
3,5-Dimethyl-1H-pyrazole		96	1.60	154	933.5	900.1	9.0
1,3,5-Trimethyl-1H-pyrazole		110	1.67	183	949.3	917.4	10.6
3,4,5-Trimethyl-1H-pyrazole		96	1.67	160	949.3	916.0	9.9
1-Methyl-3-phenyl-1H-pyrazole		144	1.00	144	932.6	900.8	15.7
1-Methyl-5-phenyl-1H-pyrazole		144	1.00	144	932.4	900.5	15.7
3,5-Diphenyl-1H-pyrazole		192	0.80	154	946.3	912.7	22.3

Pyridines		Mass		Adj. mass	PA	GB	Molecular
		(Da)	H/C	(Da)	(kJ/mol)	(kJ/mol)	Volume (Å <sup>3</sup> )
Pyridine		79	1.00	79	930.0	898.1	8.2
2-Methylpyridine		93	1.17	109	949.1	917.3	9.7
3-Methylpyridine		93	1.17	109	943.4	911.6	9.7
4-Methylpyridine		93	1.17	109	947.2	915.3	9.7
4-Vinylpyridine		105	1.00	105	944.1	912.3	11.2
2-Ethylpyridine		107	1.29	138	952.4	920.6	11.3
3-Ethylpyridine		107	1.29	138	947.4	915.5	11.3
4-Ethylpyridine		107	1.29	138	951.1	919.2	11.3
2,3-Dimethylpyridine		107	1.29	138	958.9	927.0	11.3
2,4-Dimethylpyridine		107	1.29	138	962.9	930.8	11.3
2,5-Dimethylpyridine		107	1.29	138	958.8	926.9	11.3
2,6-Dimethylpyridine		107	1.29	138	963.0	931.1	11.3
3,4-Dimethylpyridine		107	1.29	138	957.3	925.5	11.3
3,5-Dimethylpyridine		119	1.13	134	955.4	923.5	12.7
4-Isopropylpyridine		121	1.38	166	955.7	923.8	12.9
2-Propylpyridine		121	1.38	166	955.7	923.8	12.9
2,6-Diethylpyridine		135	1.44	195	972.3	940.4	14.4
4-tert-Butylpyridine		135	1.44	195	957.7	925.8	14.4
2-tert-Butylpyridine		135	1.44	195	961.7	929.8	14.4
4-Phenylpyridine		155	0.82	127	939.7	907.8	17.0
2-Hexylpyridine		163	1.55	252	963.6	931.7	17.6
2,4-Di-tert-butylpyridine		191	1.62	309	983.8	952.0	20.7
2,6-Di-tert-butylpyridine		191	1.62	309	982.9	951.0	20.7

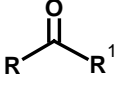
Saturated Esters		Mass		Adj. mass	PA	GB	Molecular
		(Da)	H/C	(Da)	(kJ/mol)	(kJ/mol)	Volume (Å <sup>3</sup> )
Methylformate		44	2.00	88	782.5	751.5	4.0
Ethylformate		74	2.00	148	799.4	768.4	6.5
Methylacetate		74	2.00	148	821.6	790.7	6.5
Propylformate		88	2.00	176	804.9	773.9	8.1
Isopropylformate		88	2.00	176	811.3	780.3	8.1
Ethylacetate		88	2.00	176	835.7	804.7	8.1
Methylpropanoate		88	2.00	176	830.2	799.2	8.1
Butylformate		102	2.00	204	806.0	775.0	9.6
Propylacetate		102	2.00	204	836.6	805.6	9.6
Isopropylacetate		102	2.00	204	836.6	805.6	9.6
Methylbutanoate		102	2.00	204	836.4	805.4	9.6
Methylisobutanoate		102	2.00	204	836.6	805.7	9.6
Methyl2,2-dimethylpropanoate		116	2.00	232	845.2	814.2	11.2

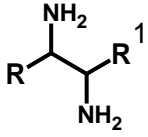
Methylcyclohexanecarboxylate	126	1.75	221	846.2	815.3	13.3
Methylcyclopropanecarboxylate	100	1.60	160	842.1	811.2	9.5


Unsaturated Esters		Mass		Adj. mass	PA	GB	Molecular
		(Da)	H/C	(Da)	(kJ/mol)	(kJ/mol)	Volume (Å <sup>3</sup> )
Methyltrans-2-butenolate		100	1.60	160	851.3	820.4	9.5
Methylbenzoate		136	1.00	136	850.5	819.5	13.8
Methyl2-methylbenzoate		150	1.11	167	858.3	827.3	15.4
Methyl3-methylbenzoate		150	1.11	167	857.7	826.8	15.4
Methyl4-methylbenzoate		150	1.11	167	861.5	830.6	15.4
Methyl4-hydroxybenzoate		152	1.00	152	863.4	832.5	14.7
Methyl3-hydroxybenzoate		152	1.00	152	850.0	819.1	14.7
Methyl4-formylbenzoate		164	0.89	146	832.9	801.9	16.2
Methyl4-methoxybenzoate		166	1.11	184	870.6	839.6	16.3
Methyl3-methoxybenzoate		134	1.11	149	856.7	825.8	14.5
Methyl2,5-dimethylbenzoate		148	1.20	178	864.7	833.7	16.1
Methyl2,4-dimethylbenzoate		148	1.20	178	868.2	837.2	16.1
Methyl3,5-dimethylbenzoate		148	1.20	178	864.3	833.4	16.1
Methyl2,4,6-trimethylbenzoate		160	1.27	204	866.3	835.3	17.4
Dimethylterephthalate		130	1.00	130	843.2	812.3	15.0
Dimethylisophthalate		146	1.00	146	843.5	814.3	15.9
4-Acetylphenylacetate		146	1.00	146	853.2	821.3	15.9
Vinylacetate		86	1.50	129	813.9	782.9	7.9
Methylacrylate		86	1.50	129	825.8	794.8	7.9
Methylmethacrylate		100	1.60	160	831.4	800.5	9.5

Alkyl Ethers		Mass		Adj. mass	PA	GB	Molecular
		(Da)	H/C	(Da)	(kJ/mol)	(kJ/mol)	Volume (Å <sup>3</sup> )
Dimethylether		46	3.00	138	792.0	764.5	4.2
Ethylmethylether		60	2.67	160	808.6	781.2	5.7
Dipentylether		148	1.20	178	852.7	825.3	16.1
Diethylether		74	2.50	185	828.4	801.0	7.3
Methylpropylether		74	2.50	185	814.9	785.7	7.3
Butyl methylether		88	2.40	211	820.3	791.2	8.9
Methyltert-butylether		88	2.40	211	841.6	812.4	8.9
Ethylisopropylether		88	2.40	211	842.7	813.5	8.9
Isopropylmethylether		90	2.50	225	826.3	797.1	8.2
tert-Butylethylether		102	2.33	238	856.0	826.9	10.4
tert-Butylisopropylether		116	2.29	265	870.7	841.5	12.0
Dipropylether		102	2.33	238	837.9	810.5	10.4
Diisopropylether		102	2.33	238	855.5	828.1	10.4
Dibutylether		130	2.25	293	845.7	818.3	13.6
Di-sec-butylether		130	2.25	293	865.9	838.5	13.6

Di-tert-butylether	178	2.25	401	887.4	860.0	16.3
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Saturated Ketones		Mass		Adj. mass	PA	GB	Molecular
		(Da)	H/C	(Da)	(kJ/mol)	(kJ/mol)	Volume (Å <sup>3</sup> )
5-Nonanone		142	2.00	284	853.7	821.9	15.0
Di-tert-butylketone		142	2.00	284	861.3	831.5	15.0
2,4-Dimethyl-3-pentanone		114	2.00	228	850.3	820.5	11.9
3,3-Dimethyl-2-butanone		116	2.00	232	840.1	808.2	11.2
2,2,4-Trimethyl-3-pentanone		128	2.00	256	856.9	825.0	13.4
2-Butanone		72	2.00	144	827.3	795.5	7.2
2-Pentanone		86	2.00	172	832.7	800.9	8.7
3-Pentanone		86	2.00	172	836.8	807.0	8.7
3-Methyl-2-butanone		86	2.00	172	836.3	804.4	8.7
3-Hexanone		100	2.00	200	843.2	811.3	10.3
4-Heptanone		114	2.00	228	845.0	815.3	11.9
Acetone		58	2.00	116	812.0	782.1	5.6
Cyclobutanone		70	1.50	105	802.5	772.7	7.0
Cyclopentanone		84	1.60	134	823.7	794.0	8.6
Cyclohexanone		98	1.67	163	841.0	811.2	10.2
Cycloheptanone		112	1.71	192	845.6	815.9	11.7
4-Methylcyclohexanone		128	1.71	219	844.9	813.0	12.6
Cyclooctanone		126	1.75	221	849.4	819.6	13.3
1-Cyclohexylethanone		142	1.75	249	841.4	809.5	14.2
Cyclononanone		172	1.78	306	852.6	822.8	16.7

Diamines		Mass		Adj. mass	PA	GB	Molecular
		(Da)	H/C	(Da)	(kJ/mol)	(kJ/mol)	Volume (Å <sup>3</sup> )
1,2-Ethanediamine		60	4.00	240	951.6	912.5	4.7
1,3-Propanediamine		74	3.33	247	987.0	940.0	6.3
1,4-Butanediamine		88	3.00	264	1005.6	954.3	7.8
1,5-Pentanediamine		102	2.80	286	999.6	946.2	9.4
1,2-Benzenediamine		108	1.33	144	896.5	865.8	10.4
1,3-Benzenediamine		108	1.33	144	929.9	899.2	10.4
1,4-Benzenediamine		108	1.33	144	905.9	874.0	10.4
Triethylenediamine		112	2.00	224	963.4	934.6	10.7
1,6-Hexanediamine		116	2.67	309	999.5	946.2	11.0
1,7-Heptanediamine		130	2.57	334	998.5	944.9	12.5
1,8-Naphthalenediamine		158	1.00	158	944.5	912.1	16.3

Primary Amines		Mass		Adj. mass	PA	GB	Molecular
		(Da)	H/C	(Da)	(kJ/mol)	(kJ/mol)	Volume (Å <sup>3</sup> )

Methylamine	31	5.00	155	899.0	864.5	2.4
Ethylamine	45	3.50	158	912.0	878.0	4.0
Cyclopropylamine	57	2.33	133	904.7	869.9	5.4
Propylamine	59	3.00	177	917.8	883.9	5.5
Isopropylamine	59	3.00	177	923.8	889.0	5.5
Butylamine	73	2.75	201	921.5	886.6	7.1
tert-Butylamine	73	2.75	201	934.1	899.9	7.1
Isobutylamine	73	2.75	201	924.8	890.8	7.1
Pentylamine	87	2.60	226	923.5	889.5	8.7
Cyclohexylamine	99	2.17	215	934.4	899.6	10.1
Hexylamine	101	2.50	253	927.5	893.5	10.2
Benzylamine	107	1.29	138	913.3	879.4	11.3
Heptylamine	115	2.43	279	923.2	889.3	11.8
Octylamine	129	2.38	306	928.9	895.0	13.4
Cyclohexanemethanamine	113	2.14	242	926.6	895.8	11.7
2,2-Dimethylpropylamine	87	2.60	226	928.3	894.0	8.7

Secondary Amines $\begin{array}{c} \text{NH} \\ \diagup \quad \diagdown \\ \text{R} \quad \text{R}^1 \end{array}$	Mass (Da)	H/C	Adj. mass (Da)	PA (kJ/mol)	GB (kJ/mol)	Molecular Volume ( $\text{\AA}^3$ )
Dimethylamine	45	3.50	158	929.5	896.5	4.0
Diethylamine	73	2.75	201	952.4	919.4	7.1
Isopropylmethylamine	73	2.75	201	952.4	919.4	7.1
Allyldimethylamine	85	2.20	187	957.8	926.8	8.6
2-Methyl-2-butanamine	87	2.60	226	937.8	903.6	8.7
Ethylisopropylamine	87	2.60	226	960.0	926.7	8.7
Dipropylamine	101	2.50	253	962.3	929.3	10.2
Diisopropylamine	101	2.50	253	971.9	938.6	10.2
Dibutylamine	129	2.38	306	968.5	935.3	13.4
Di-sec-butylamine	129	2.38	306	980.7	947.5	13.4
Diisobutylamine	129	2.38	306	958.1	925.1	13.4

Tertiary Amines $\begin{array}{c} \text{R}^1 \\   \\ \text{N} \\ / \quad \backslash \\ \text{R} \quad \text{R}^2 \end{array}$	Mass (Da)	H/C	Adj. mass (Da)	PA (kJ/mol)	GB (kJ/mol)	Molecular Volume ( $\text{\AA}^3$ )
Trimethylamine	59	3.00	177	948.9	918.1	5.5
Ethylmethylamine	73	2.75	201	960.1	929.1	7.1
Diethylmethylamine	87	2.60	226	971.0	940.0	8.7
Butylmethylamine	101	2.50	253	969.2	938.2	10.2
Isobutylmethylamine	101	2.50	253	968.7	937.8	10.2
Triethylamine	101	2.50	253	981.8	951.0	10.2
Methyldipropylamine	115	2.43	279	983.5	950.9	11.8
Diethylpropylamine	115	2.43	279	978.8	947.9	11.8
Cyclohexyldimethylamine	127	2.13	270	983.6	952.6	13.3

Tripropylamine	143	2.33	334	991.0	960.1	14.9
Tributylamine	185	2.25	416	998.5	967.6	19.6

Alcohols $R-OH$	Mass (Da)	H/C	Adj. mass (Da)	PA (kJ/mol)	GB (kJ/mol)	Molecular Volume ( $\text{\AA}^3$ )
Methanol	16	4.00	64	754.3	724.5	2.6
Ethanol	30	3.00	90	776.4	746.0	4.2
1-Propanol	44	2.67	117	786.5	756.1	5.7
2-Propanol	46	3.33	153	793.0	762.6	5.9
1-Butanol	58	2.50	145	789.2	758.9	7.3
2-Butanol	58	2.50	145	815.7	784.6	7.3
2-Methyl-1-propanol	58	2.50	145	793.7	762.2	7.3
2-Methyl-2-propanol	58	2.50	145	802.6	772.2	7.3
2,2-Dimethyl-1-propanol	72	2.40	173	795.5	765.2	8.9
Cyclohexanemethanol	98	2.00	196	802.1	771.7	11.9

Carboxylic Acids $R-C(=O)OH$	Mass (Da)	H/C	Adj. mass (Da)	PA (kJ/mol)	GB (kJ/mol)	Molecular Volume ( $\text{\AA}^3$ )
Formic acid	14	2.00	28	742.0	710.3	3.4
Acetic acid	28	2.00	56	783.7	752.8	4.9
Propanoic acid	42	2.00	84	797.2	766.2	6.5
Methacrylic acid	54	1.50	81	816.7	785.7	7.9
Cyclopropanecarboxylic acid	54	1.50	81	821.4	790.4	7.9
3-Methyl-2-butenic acid	68	1.60	109	822.9	791.9	9.5
cis-2-Methyl-2-butenic acid	68	1.60	109	822.5	791.5	9.5
Cyclobutanecarboxylic acid	68	1.60	109	817.4	786.4	9.5
Cyclopentanecarboxylic acid	82	1.67	137	817.4	786.4	11.1
Benzoic acid	90	0.86	77	821.1	790.1	12.3
Cyclohexanecarboxylic acid	96	1.71	165	823.8	792.8	12.6
Toluic acid	104	1.00	104	829.8	798.8	13.8

**Table S2:** Hydrocarbons and oxygenated hydrocarbon compounds used for statistical analysis in Fig. 7 in the manuscript and their accompanying average polarizability values. Compounds are sorted by number of carbon. Data were taken from Ref <sup>2</sup> and references therein.

Hydrocarbons	C	H	O	Mass	H/C	AM	Polarizability (10 <sup>24</sup> cm <sup>3</sup> )
methane	1	4	0	16	4.00	64	2.59
acetylene	2	2	0	26	1.00	26	3.33
ethylene	2	4	0	28	2.00	56	4.25
ethane	2	6	0	30	3.00	90	4.47
propyne	3	4	0	40	1.33	53	6.18
propene	3	6	0	42	2.00	84	6.26
cyclopropane	3	6	0	42	2.00	84	5.66
propane	3	8	0	44	2.67	117	6.29
1-butyne	4	6	0	54	1.50	81	7.41
1,3-butadiene	4	6	0	54	1.50	81	8.64
1-butene	4	8	0	56	2.00	112	7.97
trans-2-butene	4	8	0	56	2.00	112	8.49
2-methylpropene	4	8	0	56	2.00	112	8.29
butane	4	10	0	58	2.50	145	8.20
isobutane	4	10	0	58	2.50	145	8.14
1,3-cyclopentadiene	5	6	0	66	1.20	79	8.64
1-pentyne	5	8	0	68	1.60	109	9.12
trans-1,3-pentadiene	5	8	0	68	1.60	109	10.00
isoprene	5	8	0	68	1.60	109	9.99
cyclopentane	5	10	0	70	2.00	140	9.15
1-pentene	5	10	0	70	2.00	140	9.65
2-pentene	5	10	0	70	2.00	140	9.84
pentane	5	12	0	72	2.40	173	9.99
neopentane	5	12	0	72	2.40	173	10.20
benzene	6	6	0	78	1.00	78	10.00
1-hexyne	6	10	0	82	1.67	137	10.90
2-ethyl-1,3-butadiene	6	10	0	82	1.67	137	11.80
3-methyl-1,3-pentadiene	6	10	0	82	1.67	137	11.80
2-methyl-1,3-pentadiene	6	10	0	82	1.67	137	12.10
2,3-dimethyl-1,3-butadiene	6	10	0	82	1.67	137	11.80
cyclohexene	6	10	0	82	1.67	137	10.70
cyclohexane	6	12	0	84	2.00	168	11.00
1-hexene	6	10	0	82	1.67	137	11.65
hexane	6	14	0	86	2.33	201	11.90
toluene	7	8	0	92	1.14	105	11.80
1-heptyne	7	12	0	96	1.71	165	12.80
methylcyclohexane	7	14	0	98	2.00	196	13.10
1-heptene	7	14	0	98	2.00	196	13.51

heptane	7	16	0	100	2.29	229	13.61
styrene	8	8	0	104	1.00	104	15.00
ethylbenzene	8	10	0	106	1.25	133	14.20
o-xylene	8	10	0	106	1.25	133	14.90
p-xylene	8	10	0	106	1.25	133	13.70
m-xylene	8	10	0	106	1.25	133	14.20
ethylcyclohexane	8	16	0	112	2.00	224	15.90
n-octane	8	18	0	114	2.25	257	15.90
3-methylheptane	8	18	0	114	2.25	257	15.44
2,2,4-trimethylpentane	8	18	0	114	2.25	257	15.44
a-methylstyrene	9	10	0	118	1.11	131	16.05
isopropylbenzene	9	12	0	120	1.33	160	16.00
1,3,5-trimethylbenzene	9	12	0	120	1.33	160	15.50
isopropylcyclohexane	9	18	0	126	2.00	252	17.20
nonane	9	20	0	128	2.22	284	17.36
naphthalene	10	8	0	128	0.80	102	16.50
durene	10	14	0	134	1.40	188	17.30
tert-butylbenzene	10	14	0	134	1.40	188	17.20
tert-butylcyclohexane	10	20	0	140	2.00	280	19.80
decane	10	22	0	142	2.20	312	19.10
a-methylnaphthalene	11	10	0	142	0.91	129	19.35
β-methylnaphthalene	11	10	0	142	0.91	129	19.52
<b>Oxygenated hydrocarbons</b>	<b>C</b>	<b>H</b>	<b>O</b>	<b>Mass</b>	<b>H/C</b>	<b>AM</b>	<b>Polarizability</b>
ethyleneglycol	2	6	2	62	3.00	186	5.70
propenal	3	4	1	56	1.33	75	6.38
acetone	3	6	1	58	2.00	116	6.33
allyl alcohol	3	6	1	58	2.00	116	7.65
propionaldehyde	3	6	1	58	2.00	116	6.50
propionic acid	3	6	2	74	2.00	148	6.90
ethylformate	3	6	2	74	2.00	148	6.88
methylacetate	3	6	2	74	2.00	148	6.94
dimethylcarbonate	3	6	3	90	2.00	180	7.70
2-propanol	3	8	1	60	2.67	160	7.61
1-propanol	3	8	1	60	2.67	160	6.74
ethylmethylether	3	8	1	60	2.67	160	7.93
dimethoxymethane	3	8	2	76	2.67	203	7.70
ethyleneglycolmonomethylether	3	8	2	76	2.67	203	7.44
diketene	4	4	2	84	1.00	84	8.00
crotonaldehyde	4	6	1	70	1.50	105	8.50
methacrylaldehyde	4	6	1	70	1.50	105	8.30
biacetyl	4	6	2	86	1.50	129	8.20
acetic anhydride	4	6	3	102	1.50	153	8.90
butanal	4	8	1	72	2.00	144	8.20



methylethylketone	4	8	1	72	2.00	144	8.13
trans-2,3-epoxybutane	4	8	1	72	2.00	144	8.22
ethylacetate	4	8	2	88	2.00	176	8.62
1,4-dioxane	4	8	2	88	2.00	176	10.00
p-dioxane	4	8	2	88	2.00	176	8.60
2-methyl-1,3-dioxolane	4	8	2	88	2.00	176	9.44
butyricacid	4	8	2	88	2.00	176	8.58
methylpropionate	4	8	2	88	2.00	176	8.97
ethylether	4	10	1	74	2.50	185	10.20
1-butanol	4	10	1	74	2.50	185	8.88
2-methylpropanol	4	10	1	74	2.50	185	8.92
methylpropylether	4	10	1	74	2.50	185	8.86
ethyleneglycolmonoethylether	4	10	1	74	2.50	185	9.28
acetylacetone	5	8	2	100	1.60	160	10.50
diethylketone	5	10	1	86	2.00	172	9.93
methylpropylketone	5	10	1	86	2.00	172	9.93
ethylpropionate	5	10	2	102	2.00	204	10.41
methylbutanoate	5	10	2	102	2.00	204	10.41
diethylcarbonate	5	10	3	118	2.00	236	11.30
ethylpropylether	5	12	1	88	2.40	211	10.68
tetramethylorthocarbonate	5	12	4	136	2.40	326	13.00
phenol	6	6	1	94	1.00	94	11.10
ethylacetoacetate	6	10	3	130	1.67	217	12.90
cyclohexanol	6	12	1	100	2.00	200	11.56
amylformate	6	12	2	116	2.00	232	14.20
paraldehyde	6	12	3	132	2.00	264	17.90
propylether	6	14	1	102	2.33	238	12.80
1,1-diethoxyethane	6	14	2	118	2.33	275	13.20
1,2-diethoxyethane	6	14	2	118	2.33	275	11.30
anisole	7	8	1	108	1.14	123	13.10
cyclohexylmethylether	7	14	1	114	2.00	228	13.40
2,4-dimethyl-3-pentanone	7	14	1	114	2.00	228	13.50
pentylacetate	7	14	2	130	2.00	260	14.90
acetophenone	8	8	1	120	1.00	120	15.00
phenetole	8	10	1	122	1.25	153	14.90
ethylsorbate	8	12	2	140	1.50	210	17.20
tetramethylcyclobutane-1,3-dione	8	12	2	140	1.50	210	18.60
diethylsuccinate	8	14	4	174	1.75	305	16.80
butylether	8	18	1	130	2.25	293	17.20
ethylbenzoate	9	10	2	150	1.11	167	16.90
1-naphthaldehyde	11	8	1	156	0.73	113	19.75
2-naphthaldehyde	11	8	1	156	0.73	113	20.06

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