

The Classification of Solvents by Combining Classical QSPR

Methodology with Principal Component Analysis

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Table SM 7. Classification of solvents based on the score values of (703x100) matrix

Groups	Solvents	PC-1	PC2	PC3	PC4	PC5
I Hydrocarbons (81)						
Ia. Saturated hydrocarbons	propane	-1.58	-0.16	-2.23	-0.74	-0.47
	n-butane	-1.75	-0.23	-1.91	-0.47	-0.39
	n-pentane	-1.98	-0.23	-1.79	-0.16	-0.17
	n-hexane	-2.26	-0.26	-1.63	0.28	0.05
	n-heptane	-2.13	-0.24	-1.47	0.37	0.14
	n-octane	-2.19	-0.33	-1.20	0.49	0.36
	n-nonane	-2.24	-0.36	-1.01	0.71	0.61
	n-decane	-2.37	-0.40	-0.88	0.91	0.85
	n-undecane	-2.42	-0.46	-0.68	1.11	1.13
	n-dodecane	-2.54	-0.47	-0.54	1.31	1.33
	n-tridecane	-2.60	-0.53	-0.35	1.48	1.63
	n-tetradecane	-2.73	-0.58	-0.20	1.68	1.89
	n-pentadecane	-2.80	-0.57	-0.02	1.87	2.18
	hexadecane	-2.93	-0.61	0.16	2.11	2.48
	n-heptadecane	-3.01	-0.65	0.35	2.30	2.80
	isobutane	-1.74	-0.23	-2.04	-0.51	-0.35
	2-methylbutane	-1.89	-0.25	-1.81	-0.17	-0.22
	2,2-dimethylbutane	-1.87	-0.29	-1.66	-0.02	0.02
	2,3-dimethylbutane	-1.88	-0.24	-1.56	0.02	-0.03
	3-methylpentane	-1.90	-0.29	-1.55	-0.02	0.03
	isohexane	-1.91	-0.31	-1.55	-0.02	-0.02
	2,3-dimethylhexane	-2.03	-0.34	-1.18	0.44	0.35
	2,4-dimethylhexane	-2.01	-0.33	-1.23	0.42	0.41
	2,2,5-trimethylhexane	-2.09	-0.39	-1.15	0.56	0.59
	2-methylheptane	-2.08	-0.37	-1.19	0.41	0.46
	3-methylheptane	-2.09	-0.39	-1.21	0.41	0.38
	isooctane	-2.06	-0.36	-1.32	0.42	0.26
	cyclopentane	-1.75	-0.02	-1.55	-0.16	-0.56
	methylcyclopentane	-1.77	-0.17	-1.38	0.00	-0.34
	cyclohexane	-2.13	-0.07	-1.43	0.52	-0.46
	methylcyclohexane	-1.94	-0.24	-1.17	0.28	-0.31
	1,3-dimethylcyclohexane	-1.94	-0.27	-1.02	0.39	-0.08
	t-butylcyclohexane	-2.01	-0.34	-0.71	0.80	0.21
	cycloheptane	-1.97	-0.15	-1.21	0.29	-0.33
	cyclooctane	-2.02	-0.15	-0.99	0.54	-0.18
	cis-decahydronaphthalene	-2.07	-0.18	-0.60	0.89	-0.08

	perhydrofluorene	-2.22	-0.23	-0.19	1.40	0.43
	Min Ia	-3.01	-0.65	-2.23	-0.74	-0.56
	Max Ia	-1.58	-0.02	0.35	2.30	2.80
Ib. Unsaturated hydrocarbons	propene	-1.06	0.46	-1.51	-1.05	-1.15
	1-butene	-1.19	0.39	-1.26	-0.82	-0.94
	1-pentene	-1.34	0.31	-1.07	-0.60	-0.74
	isopentene	-1.32	0.34	-1.09	-0.55	-0.74
	1-hexene	-1.46	0.30	-0.89	-0.30	-0.49
	2-ethyl-1-hexene	-1.68	0.17	-0.52	0.11	-0.14
	1-heptene	-1.56	0.21	-0.68	-0.09	-0.31
	1-octene	-1.68	0.17	-0.53	0.16	-0.07
	cis-2-octene	-1.74	0.10	-0.44	0.14	-0.23
	cyclohexene	-1.44	0.37	-0.63	-0.26	-1.09
	cis-cyclooctene	-1.61	0.31	-0.33	0.21	-0.80
	alpha-pinene	-1.65	0.23	0.04	0.52	-0.63
	benzene	-0.92	1.34	-0.40	0.46	-1.11
	toluene	-0.94	1.14	-0.21	0.51	-0.87
	o-xylene	-1.03	0.96	0.07	0.56	-0.98
	m-xylene	-1.12	0.91	0.03	0.57	-0.86
	p-xylene	-1.15	1.00	0.02	0.64	-0.96
	ethyl benzene	-1.07	0.93	0.03	0.58	-0.86
	n-propylbenzene	-1.20	0.82	0.18	0.69	-0.71
	t-butylbenzene	-1.21	0.87	0.24	0.84	-0.47
	mesitylene	-1.26	0.81	0.14	0.79	-0.80
	1,2,3,4-tetramethylbenzene	-1.31	0.84	0.43	0.93	-0.69
	1,2,3,5-tetramethylbenzene	-1.32	0.81	0.39	0.94	-0.67
	cyclohexylbenzene	-1.39	0.83	0.63	1.23	-0.21
	pentadecylbenzene	-2.61	0.29	2.39	3.22	3.06
	p-cymene	-1.37	0.73	0.30	0.86	-0.60
	cumene	-1.15	0.87	0.09	0.69	-0.65
	styrene	-1.01	1.16	0.09	0.98	-0.97
	alpha-methylstyrene	-0.97	1.12	0.28	0.84	-0.87
	p-methylstyrene	-1.01	1.05	0.28	0.77	-0.89
	1-methylnaphthalene	-0.96	1.25	0.74	1.38	-0.86
	tetralin	-1.18	0.88	0.44	0.81	-0.86
	1,4-cyclohexadiene	-1.15	0.84	-0.44	-0.02	-1.25
	1,5-cyclooctadiene	-1.41	0.70	-0.11	0.40	-0.93
	dicyclopentadiene	-1.29	0.69	0.45	0.64	-0.93
	(E,Z,Z)-1,5,9-cyclododecatriene	-1.69	0.51	0.53	1.08	-0.35
	1,3,5,7-cyclooctatetraene	-1.31	1.06	0.16	0.78	-1.65
	1-hexyne	-1.10	0.71	-0.83	-0.26	-0.05
	2-heptyne	-1.53	0.51	-0.63	0.07	-0.27
	1-octyne	-1.36	0.56	-0.53	0.16	0.38
	2-octyne	-1.64	0.46	-0.48	0.30	-0.01
	1-nonyne	-1.50	0.47	-0.38	0.35	0.63
	phenyl acetylene	-0.56	1.65	0.16	0.57	-0.76
	diphenylmethane	-1.19	1.20	0.73	1.78	-0.16
	Min Ib	-2.61	0.10	-1.51	-1.05	-1.65
	Max Ib	-0.56	1.65	2.39	3.22	3.06
	Min I	-3.01	-0.65	-2.23	-1.05	-1.65

	Max I	-0.56	1.65	2.39	3.22	3.06
II Halohydrocarbons (80)						
IIa. Chloro hydrocarbons						
chloromethane		0.05	1.39	-1.49	-0.81	-0.45
trimethylchloromethane		-0.76	0.77	-0.85	-0.55	0.02
ethyl chloride		-0.34	0.96	-1.18	-0.86	-0.40
n-propyl chloride		-0.56	0.79	-0.97	-0.70	-0.18
isopropyl chloride		-0.55	0.85	-1.02	-0.69	-0.22
n-butyl chloride		-0.72	0.73	-0.80	-0.46	0.05
1-chloro-2,2-dimethylpropane		-0.83	0.66	-0.72	-0.23	0.17
propargyl chloride		0.31	1.98	-0.80	-0.83	-0.10
2-chlorobutane		-0.73	0.69	-0.82	-0.50	-0.07
2-chloropentane		-0.88	0.60	-0.64	-0.30	0.14
1-chlorohexane		-0.96	0.56	-0.48	-0.02	0.45
1-chloroheptane		-1.12	0.48	-0.33	0.16	0.64
1-chlorodecane		-1.43	0.34	0.12	0.74	1.37
chlorocyclohexane		-0.89	0.71	-0.37	-0.02	-0.03
chlorobenzene		-0.35	1.73	0.15	0.47	-0.76
benzyl chloride		-0.23	1.74	0.38	0.42	-0.40
p-chlorotoluene		-0.26	1.58	0.40	0.33	-0.59
1-chloronaphthalene		-0.41	1.87	1.00	1.43	-0.56
dichloromethane		0.17	1.79	-1.38	-0.26	-0.31
1,1-dichloroethane		-0.02	1.51	-1.04	-0.35	-0.28
1,2-dichloroethane		0.01	1.62	-1.09	-0.19	-0.20
1,2-dichloropropane		-0.16	1.31	-0.78	-0.34	0.02
1,3-dichloropropane		-0.25	1.40	-0.86	-0.04	0.03
2,2-dichloropropane		-0.28	1.40	-0.83	-0.31	0.06
1,4-dichlorobutane		-0.58	1.29	-0.78	0.36	0.12
1,10-dichlorodecane		-1.14	0.82	0.40	1.06	1.80
1,1-dichloroethene		-0.07	1.73	-1.13	-0.23	-1.17
cis-dichloroethylene		0.12	1.88	-0.81	-0.09	-0.89
trans-dichloroethylene		-0.16	1.95	-1.04	0.16	-0.93
o-dichlorobenzene		-0.20	1.87	0.15	0.63	-0.94
m-dichlorobenzene		-0.25	2.01	0.21	1.02	-0.79
p-dichlorobenzene		-0.34	2.01	0.12	1.19	-0.85
chloroform		0.17	1.94	-1.37	0.82	-0.99
1,1,1-trichloroethane		-0.02	1.80	-1.08	0.14	-0.26
1,1,2-trichloroethane		0.06	1.90	-0.90	0.37	-0.26
trichloroethylene		-0.35	1.61	-1.01	0.70	-1.57
1,2,3-trichloropropane		-0.02	1.72	-0.67	0.22	0.21
1,2,3-trichlorobenzene		-0.21	1.98	0.23	1.14	-1.08
1,3,4-trichlorobenzene		-0.33	2.00	0.10	1.28	-1.16
carbon tetrachloride		-1.04	1.73	-1.28	1.21	-1.01
1,1,2,2-tetrachloroethane		0.06	2.14	-0.75	0.84	-0.22
tetrachloroethylene		-1.05	1.55	-0.89	0.90	-1.67
1,2,3,4-tetrachlorobenzene		-0.28	2.10	0.25	1.59	-1.18
pentachloroethane		-0.30	1.92	-0.96	1.72	-0.60
hexachloro-1,3-butadiene		-1.26	1.64	-0.12	1.94	-1.38
hexachloropropene		-0.70	2.00	-0.36	1.37	-1.07
hexachlorocyclopentadiene		-0.78	1.98	0.38	1.71	-1.43

	Min IIa	-1.43	0.34	-1.49	-0.86	-1.67
	Max IIa	0.31	2.14	1.00	1.94	1.80
IIb. Bromo hydrocarbons	bromoethane	-0.44	0.52	-0.19	-0.55	-1.24
	1-bromopropane	-0.64	0.37	-0.09	-0.33	-1.00
	2-bromopropane	-0.61	0.47	-0.12	-0.34	-0.97
	1-bromobutane	-0.80	0.32	-0.01	-0.09	-0.71
	2-bromobutane	-0.73	0.36	0.03	-0.15	-0.74
	1-bromopentane	-0.93	0.21	0.19	0.11	-0.50
	2-bromo octane	-1.28	0.04	0.60	0.66	0.23
	bromobenzene	-0.35	1.52	0.48	0.80	-1.23
	1-bromonaphthalene	-0.44	1.32	1.38	1.53	-1.00
	dibromomethane	-0.08	0.95	-0.26	-0.08	-2.03
	1,2-dibromoethane	-0.39	1.35	-0.10	0.70	-1.25
	1,2-dibromopropane	-0.55	1.05	0.14	0.58	-0.91
	o-dibromobenzene	-0.25	1.08	1.12	0.88	-1.48
	m-dibromobenzene	-0.44	1.20	0.93	1.07	-1.45
	2,5-dibromotoluene	-0.58	1.41	0.88	1.17	-1.02
	tribromomethane	-0.36	0.90	-0.05	0.75	-2.26
	Min IIb	-1.28	0.04	-0.26	-0.55	-2.26
	Max IIb	0.08	1.52	1.38	1.53	0.23
IIc. Iodo hydrocarbons	iodomethane	0.01	0.83	-0.15	-0.21	-1.98
	methylene iodide	0.19	1.30	0.34	0.33	-2.16
	ethyliodide	-0.39	0.45	-0.04	-0.31	-1.83
	1-iodopropane	-0.59	0.28	0.12	-0.17	-1.56
	1-iodobutane	-0.76	0.17	0.27	0.04	-1.30
	2-iodobutane	-0.77	0.19	0.28	0.00	-1.38
	iodobenzene	-0.23	1.31	0.82	0.72	-1.34
	1-iodonaphthalene	-0.29	1.23	1.75	1.42	-1.24
	Min IIc	-0.77	0.17	-0.15	-0.31	-2.16
	Max IIc	0.19	1.31	1.75	1.42	-1.24
IId. Fluoro hydrocarbons	fluorobenzene	-0.08	1.50	-0.25	0.42	-0.31
	1,2-difluorobenzene	0.55	1.49	-0.28	0.58	0.19
	1,3-difluorobenzene	0.42	1.59	-0.42	0.68	0.37
	trifluoromethyl benzene	0.93	1.85	-0.10	0.84	1.20
	Min IId	-0.08	1.49	-0.42	0.42	-0.31
	Max IId	0.93	1.85	-0.10	0.84	1.20
IIe. Mixed halo hydrocarbons	trichlorofluoromethane	0.01	1.69	-1.48	0.92	-0.31
	bromotrichloromethane	-0.03	1.47	-1.09	2.18	-1.61
	1,1,1-trichlorotrifluoroethane	0.36	1.73	-1.80	1.20	0.64
	1,2,2-trichlorotrifluoroethane	0.35	1.83	-1.63	1.46	0.71
	1,2-dichlorohexafluorocyclobutane	0.90	1.86	-2.01	2.04	1.70
	Min IIe	-0.03	1.47	-2.01	0.92	-1.61
	Max IIe	0.90	1.86	-1.09	2.18	1.70
	Min II	-1.43	0.04	-2.01	-0.86	-2.26
	Max II	0.93	2.14	1.75	2.18	1.80

III. Ethers (58)

III. Saturated, unsaturated and cyclic ethers	dimethyl ether	-0.43	-0.15	-1.72	-1.40	-0.09
	diethyl ether	-0.96	-0.57	-1.05	-0.92	0.11
	di-n-propyl ether	-1.08	-0.53	-0.59	-0.48	0.39
	diisopropylether	-1.08	-0.51	-0.61	-0.48	0.40

di-n-butylether	-1.30	-0.55	-0.33	0.11	0.69
ethyl n-butyl ether	-1.03	-0.47	-0.61	-0.41	0.42
di-t-butyl ether	-1.22	-0.53	-0.29	-0.15	0.58
n-butyl methyl ether	-0.88	-0.44	-0.84	-0.61	0.26
t-butyl methyl ether	-0.85	-0.41	-0.89	-0.69	0.28
di-n-pentyl ether	-1.50	-0.73	0.07	0.40	1.32
ethyl isopropyl ether	-0.87	-0.48	-0.80	-0.63	0.18
di-n-hexyl ether	-1.69	-0.78	0.42	0.83	1.89
hexyl methyl ether	-1.10	-0.55	-0.47	-0.17	0.69
tert-amyl methyl ether	-0.96	-0.47	-0.63	-0.47	0.31
diallyl ether	-0.25	0.55	0.03	-0.42	0.11
ethyl vinyl ether	-0.29	0.23	-0.54	-1.26	-0.31
n-butyl vinyl ether	-0.54	0.08	-0.14	-0.72	0.10
isobutyl vinyl ether	-0.61	0.01	-0.09	-0.81	-0.06
ethyldine diethyl ether	-0.75	-0.48	-0.25	-0.44	0.58
diglyme	-0.57	-0.20	-0.24	-0.08	1.19
diethylene glycol diethyl ether	-0.96	-0.28	0.16	0.39	1.49
triethylene glycol dimethyl ether	-0.94	-0.15	-0.03	0.72	2.06
dimethoxymethane	-0.13	-0.17	-1.02	-1.04	0.22
diethoxymethane	-0.57	-0.46	-0.38	-0.71	0.35
1,2-dimethoxyethane	-0.60	-0.09	-0.88	-0.43	0.43
1,1,2-triethoxyethane	-0.77	-0.68	0.40	-0.09	1.16
diphenyl ether	-0.45	1.17	1.26	1.48	0.14
dibenzyl ether	-0.44	0.97	1.56	1.45	0.75
o-methoxytoluene	-0.35	0.61	0.74	0.15	-0.56
propoxybenzene	-0.40	0.64	0.84	0.32	-0.11
anisole	-0.19	1.20	0.35	0.25	-0.50
phenetole	-0.36	0.97	0.58	0.26	-0.30
veratrole	-0.23	0.76	0.79	0.36	-0.24
furan	0.27	0.90	-1.17	0.98	-1.25
THF	-0.25	-0.10	-0.57	-1.38	0.14
2-methylfuran	0.05	0.58	-0.54	0.27	-1.14
2-methyltetrahydrofuran	-0.64	-0.22	-0.78	-0.82	0.03
2,5-Dimethyltetrahydrofuran	-0.79	-0.34	-0.59	-0.57	0.19
2,2,5,5-tetramethyltetrahydrofuran	-1.02	-0.37	-0.27	-0.26	0.55
dihydropyran	-0.21	0.35	-0.01	-0.79	-0.70
tetrahydropyran	-0.64	-0.33	-0.69	-0.72	0.13
tetrahydro-3-methylpyran	-0.77	-0.35	-0.64	-0.42	0.17
oxane	0.04	0.58	-1.88	-1.37	0.24
propylene oxide	-0.12	0.28	-1.45	-1.04	0.26
oxepane	-0.84	-0.32	-0.56	-0.39	0.10
styrene oxide	0.09	1.23	0.46	0.27	-0.01
1,8-Cineole	-1.08	-0.48	0.25	0.18	0.46
epichlorohydrin	0.27	1.05	-1.09	-0.29	0.18
bis(2-chloroethyl) ether	-0.12	0.91	-0.46	0.26	0.29
1,4-dioxane	-0.48	0.23	-1.07	-0.44	-0.32
5-acetyl-5-methyl-1,3-dioxane	0.72	-0.88	0.03	0.44	0.41
3,3-bischloromethyloxetane	0.19	1.05	-0.26	0.17	0.45
1,3-dioxolane	0.00	0.34	-1.09	-0.76	0.23
2-methyl-1,3-dioxolane	-0.26	0.15	-0.90	-0.56	0.31

4-methyl-1,3-dioxolane	-0.23	0.15	-0.87	-0.63	0.36
2-phenyl-1,3-dioxolane	-0.04	0.92	0.76	0.45	0.27
4-chloromethyl-1,3-dioxolane	0.28	0.81	-0.55	-0.25	0.47
2-methoxy-1,3-dioxolane	-0.04	0.19	-1.01	-0.15	0.77
Min III	-1.69	-0.88	-1.88	-1.40	-1.25
Max III	0.72	1.23	1.56	1.48	2.06

IV. Esters (67)

IV. Esters and polyesters	methyl formate	1.10	0.88	-1.46	-1.64	0.83
	ethyl formate	0.82	0.69	-1.01	-1.42	0.86
	n-propyl formate	0.61	0.54	-0.77	-1.20	1.05
	butyl formate	0.43	0.46	-0.57	-0.93	1.22
	benzyl formate	0.81	1.17	0.59	-0.02	0.75
	trimethyl orthoformate	0.12	-0.26	-0.58	-0.85	0.83
	methyl acetate	0.25	0.69	-1.23	-1.05	0.84
	ethyl acetate	-0.13	0.39	-0.80	-1.05	0.69
	n-propyl acetate	-0.10	0.51	-0.67	-0.58	1.09
	n-butyl acetate	-0.29	0.37	-0.49	-0.38	1.18
	isopropyl acetate	-0.12	0.47	-0.71	-0.59	0.95
	n-pentyl acetate	-0.35	0.37	-0.35	-0.09	1.48
	isoamyl Acetate	-0.31	0.37	-0.35	-0.12	1.45
	vinyl acetate	0.42	1.00	-0.63	-0.88	0.44
	trimethyl orthoacetate	-0.60	-0.31	-0.48	-0.33	0.68
	1,3-Benzenediol, monoacetate	2.42	0.00	0.28	1.89	0.35
	benzyl acetate	0.28	1.14	0.67	0.46	0.68
	ethyl methoxyacetate	0.04	0.38	-0.40	-0.52	1.01
	methyl chloroacetate	0.59	1.25	-0.75	-0.90	0.94
	ethyl chloroacetate	0.38	1.12	-0.49	-0.70	1.16
	methyl dichloroacetate	0.66	1.63	-0.58	-0.54	1.04
	methyl trichloroacetate	0.32	1.66	-0.58	-0.21	0.68
	ethyl trichloroacetate	0.14	1.50	-0.31	-0.06	0.83
	ethyl trifluoroacetate	1.48	1.62	-1.13	-0.21	2.21
	ethyl acetoacetate	0.93	0.10	0.30	-0.88	1.45
	methyl propionate	0.02	0.59	-0.93	-0.75	0.80
	ethyl propionate	-0.16	0.46	-0.63	-0.54	0.95
	pentyl propionate	-0.57	0.24	-0.13	0.12	1.60
	diethyl malonate	0.04	0.72	-0.09	-0.31	2.09
	methyl valerianate	-0.30	0.33	-0.57	-0.33	1.16
	ethyl butanoate	-0.32	0.35	-0.47	-0.35	1.12
	propyl butanoate	-0.47	0.28	-0.29	-0.13	1.34
	isobutyl isobutanoate	-0.61	0.20	-0.15	-0.01	1.40
	isoamyl isopentanoate	-0.78	0.11	0.15	0.44	1.98
	methyl butyrate	-0.14	0.45	-0.76	-0.55	0.99
	methyl isobutyrate	-0.15	0.47	-0.72	-0.57	0.95
	ethyl octanoate	-0.85	0.04	0.22	0.51	1.97
	ethyl decanoate	-1.08	-0.06	0.58	0.94	2.48
	methyl benzoate	0.34	1.33	0.53	0.32	0.59
	butyl benzoate	-0.03	1.03	1.08	0.70	1.23
	n-pentyl benzoate	-0.15	0.97	1.27	0.89	1.52
	benzyl benzoate	0.10	1.37	1.64	1.60	1.51
	ethyl o-ethylbenzoate	0.17	1.21	0.73	0.40	0.73

methyl hydroxybenzoate	1.53	0.14	0.43	1.48	-0.03
methyl caproate	-0.44	0.25	-0.36	-0.10	1.36
ethyl cinnamate	0.17	1.21	1.26	0.83	1.04
methyl acrylate	0.40	1.01	-0.70	-0.77	0.51
ethyl acrylate	0.24	0.88	-0.43	-0.58	0.70
methyl methacrylate	0.17	0.81	-0.33	-0.79	0.49
dimethyl adipate	-0.26	0.77	-0.31	0.39	2.45
diethyl maleate	0.36	0.87	0.46	-0.20	1.96
ethyl propiolate	0.90	1.21	-1.25	0.30	0.70
ethyl lactate	1.14	-0.74	-0.64	0.46	0.70
diethyl phthalate	0.21	1.21	1.40	0.51	2.12
dibutyl oxalate	-0.55	0.68	0.29	0.96	2.65
dimethyl phthalate	0.25	1.36	0.86	0.79	1.36
ethyl Salicylate	1.50	-0.05	0.66	1.61	0.20
phenyl Salicylate	1.27	0.58	1.43	2.45	0.95
nonyl phenol ethoxylate	0.18	-0.09	2.82	1.82	2.93
dimethyl carbonate	0.33	0.84	-1.41	-0.58	1.20
diethyl carbonate	-0.15	0.48	-0.83	-0.17	1.32
propylene carbonate	1.31	0.92	-0.92	-1.25	1.62
ethylene carbonate	1.51	1.15	-1.27	-1.27	1.55
beta-propiolactone	1.19	1.21	-1.15	-1.29	0.94
4-butyrolactone	1.05	0.82	-0.65	-1.13	0.85
gama-caprolactone	0.49	0.51	-0.17	-0.82	0.99
delta-valerolactone	0.67	0.63	-0.36	-1.05	0.85
Min IV	-1.08	-0.74	-1.46	-1.64	-0.03
Max IV	2.42	1.66	2.82	2.45	2.93

V. Aldehydes, ketones and amides (84)

Va. Aldehydes	acetaldehyde	0.90	0.43	-1.24	-2.04	0.20
	propionaldehyde	0.58	0.26	-0.74	-1.69	0.26
	n-butyraldehyde	0.36	0.12	-0.45	-1.39	0.41
	acrolein	1.01	0.59	-0.33	-1.29	-0.19
	crotonaldehyde	0.89	0.57	0.01	-1.31	0.04
	benzaldehyde	0.61	1.11	0.60	-0.06	0.04
	p-methoxybenzaldehyde	0.99	0.76	1.20	-0.51	0.49
	isobutyraldehyde	0.32	0.12	-0.55	-1.43	0.34
	3-methylbutanal	0.21	0.01	-0.28	-1.18	0.61
	hexanal	0.05	-0.16	0.06	-0.92	0.79
	heptanal	-0.10	-0.31	0.29	-0.72	0.99
	octanal	-0.22	-0.44	0.51	-0.53	1.19
	2-butenal	0.91	0.57	0.01	-1.32	0.06
	Min Va	-0.22	-0.44	-1.24	-2.04	-0.19
	Max Va	1.01	1.11	1.20	-0.06	1.19

Vb. Ketones	acetone	0.39	0.38	-0.84	-1.85	0.57
	diethyl ketone	-0.10	-0.06	-0.13	-1.21	0.33
	methyl isopropyl ketone	0.06	-0.12	-0.20	-1.28	0.42
	dibutyl Ketone	-0.55	-0.70	0.84	-0.43	1.22
	methyl isobutyl ketone	-0.09	-0.24	0.12	-1.06	0.49
	methyl vinyl ketone	0.69	0.51	-0.08	-1.29	-0.05
	2-butanone	0.21	0.20	-0.47	-1.59	0.38
	2-pentanone	0.09	-0.15	-0.10	-1.34	0.43

	hexanone	-0.05	-0.31	0.20	-1.04	0.58
	2-hexanone	-0.06	-0.28	0.16	-1.00	0.60
	3-hexanone	-0.28	-0.40	0.19	-1.06	0.43
	heptanone	-0.23	-0.49	0.43	-0.80	0.73
	2-heptanone	-0.21	-0.45	0.40	-0.83	0.77
	3-heptanone	-0.34	-0.52	0.39	-0.86	0.67
	4-heptanone	-0.35	-0.50	0.40	-0.84	0.66
	2-octanone	-0.31	-0.58	0.63	-0.65	0.98
	3-octanone	-0.51	-0.69	0.67	-0.65	0.80
	nonanone	-0.50	-0.76	0.88	-0.42	1.14
	2-nonanone	-0.46	-0.73	0.86	-0.45	1.21
	2-decanone	-0.55	-0.84	1.06	-0.26	1.42
	2-undecanone	-0.67	-0.97	1.28	-0.10	1.65
	2-dodecanone	-0.77	-1.08	1.49	0.11	1.92
	3,3-dimethyl-2-butanone	-0.05	-0.21	0.03	-1.13	0.65
	2,4-dimethyl-3-pentanone	-0.39	-0.40	0.29	-0.88	0.61
	2,2,4,4-tetramethyl-3-pentanone	-0.58	-0.55	0.62	-0.54	0.96
	2,6-dimethyl-4-heptanone	-0.50	-0.70	0.70	-0.47	1.09
	alpha-isophorone	0.32	0.06	1.16	-0.54	0.63
	1,1,1-trichloroacetone	0.69	1.41	-0.12	-0.57	0.47
	1,1,1-trichlorotrifluoroacetone	1.00	2.06	-1.33	0.92	1.29
	acetoacetone	0.76	0.53	-0.02	-0.84	0.92
	hexachloroacetone	-0.31	1.59	-0.51	1.17	-0.19
	phenylacetone	0.34	0.75	0.97	-0.07	0.36
	acetophenone	0.56	0.96	0.89	-0.22	0.14
	benzophenone	0.15	1.32	1.55	1.24	0.83
	4-methoxyacetophenone	0.57	0.84	1.24	-0.15	0.66
	cyclopentanone	0.30	0.31	-0.07	-1.17	0.30
	cyclohexanone	0.13	0.27	0.17	-1.06	0.39
	2-methylcyclohexanone	0.05	-0.13	0.32	-0.87	0.48
	3-methylcyclohexanone	0.06	-0.14	0.29	-0.84	0.57
	cyclobutanone	0.57	0.49	-0.40	-1.38	0.22
	cycloheptanone	-0.02	-0.10	0.46	-0.87	0.52
	cyclooctanone	-0.19	-0.31	0.68	-0.53	0.52
	cyclononanone	-0.27	-0.32	0.82	-0.41	0.88
	cyclodecanone	-0.40	-0.44	1.03	-0.22	1.02
	cycloundecanone	-0.49	-0.62	1.23	0.01	1.11
	cyclododecanone	-0.55	-0.72	1.43	0.10	1.38
	2,6-dimethyl-4H-pyran-4-one	0.91	0.65	1.12	-1.15	0.56
	camphor	-0.18	-0.39	0.92	-0.26	0.70
	flavone	0.65	1.44	2.33	1.28	1.48
	carvone	0.27	0.13	1.38	-0.27	0.51
	anthrone	0.47	1.24	1.88	0.96	0.81
	Min Vb	-0.77	-1.08	-1.33	-1.85	-0.19
	Max Vb	1.00	2.06	2.33	1.28	1.92
Vc. Amides	formamide	2.74	-0.28	-1.51	-0.14	-0.68
	N-methylformamide	2.07	-0.34	-0.87	-1.09	-0.34
	N,N-dimethylformamide	0.95	0.08	0.20	-1.88	0.19
	N,N-diethylformamide	0.47	-0.31	0.79	-1.42	0.30
	N-methylacetamide	1.54	-0.66	-0.21	-1.26	-0.34

N,N-dimethylacetamide	0.83	-0.07	0.54	-1.66	0.33
N,N-diethylacetamide	0.36	-0.36	0.97	-1.12	0.34
N,N-dimethylpropanamide	0.46	-0.29	0.68	-1.32	0.24
N,N-dimethylchloroacetamide	1.04	0.41	0.76	-1.36	0.32
N,N-dimethylbenzamide	0.63	0.57	1.66	-0.36	0.28
N,N-diethylbenzamide	0.45	0.31	2.13	-0.05	0.69
dimethylcyanamide	0.73	0.11	-0.19	-2.06	-0.17
diethylcyanamide	0.25	-0.37	0.46	-1.63	0.09
diisopropylcyanamide	0.00	-0.59	0.89	-1.28	0.49
N,N-dimethylthioformamide	0.84	0.04	1.41	-1.46	-1.62
tetramethyl thiourea	0.71	-0.59	2.45	-1.31	-0.96
N,N'-dimethylpropyleneurea	0.69	-0.53	1.64	-1.23	0.09
1,1,3,3-tetraethylurea	-0.23	-0.94	1.98	-0.22	0.83
1,1,3,3-tetramethylurea	0.52	-0.37	1.32	-1.26	0.09
N-methylcaprolactam	0.38	-0.38	1.13	-0.98	0.35
Min Vc	-0.23	-0.94	-1.51	-2.06	-1.62
Max Vc	2.74	0.57	2.45	-0.05	0.83
Min V	-0.77	-1.08	-1.51	-2.06	-1.62
Max V	2.74	2.06	2.45	1.28	1.92

VI. Nitriles and nitro compounds (36)

VIIa. Nitriles	acetonitrile	0.78	0.71	-1.54	-1.83	0.41
	propionitrile	0.36	0.49	-1.08	-1.82	0.22
	3-methoxypropionitrile	0.51	0.20	-0.46	-1.47	0.61
	3-ethoxypropionitrile	0.26	0.01	-0.12	-1.31	0.70
	oxydipropionitrile	0.54	0.55	-0.16	-0.71	1.21
	2,2-dimethyl-propanenitrile	-0.15	0.20	-0.69	-1.38	0.66
	n-butanenitrile	0.14	0.31	-0.80	-1.50	0.37
	isobutyronitrile	0.08	0.34	-0.87	-1.56	0.39
	hexanenitrile	-0.23	-0.03	-0.17	-1.10	0.65
	nonanenitrile	-0.61	-0.41	0.50	-0.43	1.19
	dodecanenitrile	-0.95	-0.81	1.20	0.10	1.86
	undecanenitrile	-0.89	-0.69	1.07	-0.09	1.72
	pentanedinitrile	0.63	0.61	-0.36	-1.39	0.76
	n-pentadecanonitrile	-1.26	-1.12	1.88	0.70	2.72
	chloroacetonitrile	1.08	1.54	-0.84	-1.29	-0.13
	trichloroacetonitrile	0.03	1.65	-0.98	0.14	-0.42
	phenylacetonitrile	0.42	1.22	0.80	-0.27	-0.15
	acrylonitrile	0.84	0.90	-0.63	-1.73	-0.49
	valeronitrile	-0.08	0.13	-0.47	-1.33	0.47
	benzonitrile	0.49	1.36	0.52	-0.29	-0.16
	4-methoxybenzonitrile	0.82	1.04	1.17	-0.65	0.14
	4-dimethylaminobenzonitrile	0.81	0.72	2.05	-1.16	0.05
	cyclohexanecarbonitrile	-0.29	0.02	0.12	-0.78	0.31
	1-pyrrolidinecarbonitrile	0.58	-0.06	0.55	-1.61	-0.16
	1-piperidinecarbonitrile	0.34	-0.25	0.77	-1.40	-0.01
	4-morpholinecarbonitrile	0.71	0.22	0.64	-1.19	0.22
	Min VIIa	-1.26	-1.12	-1.54	-1.83	-0.49
	Max VIIa	1.08	1.65	2.05	0.70	2.72
VIb. Nitro hydrocarbons	nitromethane	1.39	1.77	-1.37	-1.39	0.75
	nitroethane	0.98	1.66	-0.96	-1.31	1.14

n-nitropropane	0.76	1.52	-0.66	-1.20	1.26
isopropyl nitrate	0.87	1.43	-0.54	-1.06	1.52
2-methyl-2-nitropropane	0.46	1.45	-0.49	-1.06	1.29
dimethylnitromethane	0.67	1.50	-0.67	-1.22	1.14
nitrocyclohexane	0.37	1.36	0.06	-0.62	1.35
nitrobenzene	1.02	2.06	0.63	-0.37	0.91
3-nitrotoluene	1.09	2.04	0.82	-0.55	1.09
2-nitrophenol	2.85	0.70	-0.21	2.07	0.25
Min VIb	0.37	0.70	-1.37	-1.39	0.25
Max VIb	2.85	2.06	0.82	2.07	1.52
Min VI			-1.26	-1.12	-1.54
Max VI			2.85	2.06	2.05
				2.07	2.72

VII. Hydroxylic compounds (125)

VIIa. Monohydric alcohols	methanol	1.42	-1.11	-2.77	0.16	-0.52
	ethanol	1.01	-1.40	-2.12	-0.01	-0.23
	n-propanol	0.79	-1.49	-1.39	0.41	-0.45
	2-propanol	0.65	-1.57	-1.61	0.06	-0.16
	n-butanol	0.71	-1.71	-1.35	0.48	-0.12
	2-butanol	0.42	-1.64	-1.14	0.15	-0.20
	tert-butanol	0.41	-1.49	-1.18	-0.10	0.09
	n-pentanol	0.48	-1.71	-0.98	0.66	0.10
	3-Pentanol	0.30	-1.71	-0.82	0.32	-0.04
	n-hexanol	0.38	-1.86	-0.72	0.86	0.25
	n-heptanol	0.23	-1.96	-0.49	1.00	0.45
	n-octanol	0.13	-2.05	-0.33	1.26	0.58
	2-octanol	-0.14	-2.04	-0.19	0.81	0.71
	2-hexanol	0.13	-1.85	-0.56	0.52	0.21
	3-hexanol	0.05	-1.76	-0.57	0.38	0.33
	1-nonanol	-0.02	-2.18	-0.08	1.33	0.88
	n-decanol	-0.13	-2.24	0.14	1.49	1.12
	undecanol	-0.23	-2.40	0.34	1.68	1.34
	dodecanol	-0.33	-2.52	0.57	1.82	1.63
	2-methyl-1-propanol	0.54	-1.64	-1.27	0.34	-0.14
	3-methyl-1-butanol	0.55	-1.75	-1.10	0.61	0.14
	3-methyl-2-butanol	0.23	-1.71	-0.85	0.30	-0.04
	2-methyl-1-butanol	0.41	-1.76	-0.92	0.50	-0.04
	2-methyl-2-pentanol	0.11	-1.76	-0.63	0.41	0.22
	3-methyl-3-pentanol	-0.02	-1.73	-0.56	0.24	0.20
	3-ethyl-3-pentanol	-0.09	-1.81	-0.27	0.48	0.29
	2,4-dimethyl-3-pentanol	-0.07	-1.75	-0.36	0.49	0.41
	sec-amyl alcohol	0.23	-1.68	-0.88	0.28	0.14
	t-amyl alcohol	0.13	-1.63	-0.81	0.11	0.05
	2-methyl-1-pentanol	0.28	-1.89	-0.67	0.71	0.08
	2-methyl-heptan-2-ol	-0.06	-2.00	-0.24	0.76	0.64
	methyl-2-pentanol	0.30	-1.75	-0.73	0.57	0.32
	3-phenyl-1-propanol	0.91	-0.34	0.54	1.50	-0.29
	3,3-dimethyl-2-butanol	0.08	-1.77	-0.65	0.41	0.10
	2-ethyl-1-hexanol	-0.09	-2.14	-0.14	0.94	0.36
	allyl alcohol	1.32	-0.66	-1.06	0.22	-0.65
	trans-2-hexenol	0.68	-1.14	-0.21	0.54	-0.25

	trans-2-heptenol	0.60	-1.33	0.01	0.78	-0.09
	trans-2-octenol	0.43	-1.47	0.25	0.91	0.09
	propargyl alcohol	1.88	-0.02	-1.48	0.54	-0.48
	2-ethoxyethanol	0.54	-1.16	-1.04	0.56	0.07
	2-butoxyethanol	0.25	-1.44	-0.56	0.90	0.54
	2-chloroethanol	1.58	-0.41	-1.46	0.90	-0.56
	cyclopentanol	0.47	-1.47	-0.83	0.49	-0.25
	cyclohexanol	0.31	-1.58	-0.55	0.56	-0.28
	2-methylcyclohexanol	0.19	-1.72	-0.30	0.67	-0.06
	cycloheptanol	0.21	-1.74	-0.38	0.80	-0.03
	cyclooctanol	0.12	-1.80	-0.12	1.02	0.13
	furfuryl alcohol	1.56	-0.38	-0.59	1.57	-1.06
	tetrahydrofurfuryl alcohol	0.64	-1.07	-0.65	0.30	0.22
	2-phenylethanol	0.95	-0.10	0.26	1.21	-0.30
	benzyl alcohol	1.17	-0.14	0.19	1.37	-0.91
	2,2,2-trichloroethanol	1.52	0.21	-0.75	1.16	-0.59
	hexafluoropropan-2-ol	2.73	0.93	-2.78	1.95	2.62
	1-methoxy-2-propanol	0.49	-1.13	-1.00	0.35	0.18
	2-methoxyethanol	0.84	-0.87	-1.44	0.56	0.07
	DL-sec-phenethyl alcohol	0.85	-0.21	0.50	1.17	-0.59
	3-ethyl-2,4-dimethyl-3-pentanol	-0.44	-2.05	0.25	0.60	0.46
Min VIIa		-0.44	-2.52	-2.78	-0.10	-1.06
Max VIIa		2.73	0.93	0.57	1.95	2.62
VIIb. Phenols	phenol	1.19	0.10	-0.18	1.76	-1.06
	o-cresol	1.04	-0.24	0.32	1.38	-1.10
	m-cresol	1.31	-0.12	0.13	1.92	-1.11
	p-Cresol	1.12	-0.19	0.16	1.50	-0.92
	2-ethylphenol	0.79	-0.41	0.63	1.24	-0.98
	m-ethylphenol	0.95	-0.34	0.47	1.47	-0.72
	4-ethylphenol	0.94	-0.33	0.49	1.38	-0.74
	2-isopropylphenol	0.73	-0.49	0.77	1.43	-0.63
	2-tert-butylphenol	0.49	-0.62	1.09	1.34	-0.63
	4-tert-butylphenol	0.75	-0.54	0.87	1.60	-0.29
	2,3-xylenol	0.82	-0.36	0.63	1.37	-0.96
	2,4-xylenol	0.79	-0.48	0.65	1.27	-1.02
	3,4-xylenol	0.93	-0.28	0.56	1.38	-0.74
	3,5-xylenol	0.96	-0.34	0.52	1.42	-0.78
	5-isopropyl-2-methyl-phenol	0.60	-0.54	1.01	1.43	-0.20
	5-methyl-2-isopropyl-1-phenol	0.41	-0.74	1.21	1.25	-0.63
	2-tert-butyl-4-methylphenol	0.30	-0.88	1.30	1.44	-0.53
	2,4-di-tert-butylphenol	-0.04	-1.24	1.89	1.81	0.07
	2,6-di-tert-butylphenol	-0.24	-1.00	2.02	1.38	0.34
	2,3,5-trimethylphenol	0.67	-0.55	0.94	1.39	-0.76
	2,3,6-trimethyl-phenol	0.48	-0.39	1.01	1.16	-0.63
	2,6-Di-tert-butyl-4-methylphenol	-0.41	-1.21	2.16	1.54	0.49
	4-fluorophenol	1.45	0.27	-0.17	1.43	-0.48
	2-chlorophenol	1.25	0.25	0.33	1.30	-1.08
	3-chlorophenol	1.55	0.54	0.13	1.83	-0.83
	4-chlorophenol	1.43	0.44	0.15	1.70	-0.92
	4-bromophenol	1.21	0.08	0.48	1.68	-1.27

	2,6-dichlorophenol	1.10	0.53	0.53	1.58	-1.04
	4-chloro-3-methylphenol	1.29	0.20	0.48	1.59	-0.86
	4-methoxyphenol	1.13	-0.12	0.49	0.97	-0.66
	2,6-dimethoxyphenol	0.79	-0.38	1.20	0.93	-0.39
	3,5-dimethoxyphenol	1.33	-0.37	0.58	1.75	-0.04
Min VIIb		-0.41	-1.24	-0.18	0.93	-1.27
Max VIIb		1.55	0.54	2.16	1.92	0.49
VIIc. Di and tri-hydroxy alcohols	diethylene glycol	1.73	-1.61	-1.21	1.57	0.23
	triethylene glycol	1.31	-1.49	-0.98	2.57	1.11
	tetraethylene glycol	1.43	-2.08	-0.14	2.72	1.76
	1,2-ethanediol	1.94	-1.10	-2.07	1.27	-0.26
	1,2-propanediol	1.77	-1.72	-1.31	0.56	-0.08
	1,3-propanediol	2.11	-1.79	-1.37	0.90	-0.18
	1,2-butanediol	1.42	-1.69	-1.12	0.55	0.31
	1,3-butanediol	1.57	-1.72	-1.15	0.92	0.15
	1,4-butanediol	1.38	-1.36	-1.60	1.68	0.23
	2,3-butanediol	1.44	-1.72	-1.02	0.52	0.20
	1,5-pentanediol	1.68	-2.04	-0.83	1.12	0.24
	glycerol	2.80	-1.87	-1.50	1.50	0.11
	dihydroxybenzene	2.10	-0.52	0.12	1.72	-1.09
Min VIIc		1.31	-2.08	-2.07	0.52	-1.09
Max VIIc		2.80	-0.52	0.12	2.72	1.76
VIID. Mixed alcohols	1-amino-2-propanol	1.54	-2.05	-0.55	0.04	-0.71
	2-amino-1-butanol	1.33	-2.52	-0.06	0.04	-0.85
	2-amino-1-hydroxybenzene	1.90	-0.41	0.31	2.21	-1.49
	3-amino-1-hydroxybenzene	2.11	-0.57	0.29	2.15	-1.36
	ethanol amine	1.70	-1.71	-1.06	0.48	-0.83
	triethanolamine	2.48	-2.41	-0.34	2.74	0.15
	2-cyanoethanol	2.28	-0.64	-1.75	0.82	-0.17
	4-cyanophenol	2.10	0.34	-0.02	1.80	-0.48
Min VIIId		1.33	-2.52	-1.75	0.04	-1.49
Max VIIId		2.48	0.34	0.31	2.74	0.15
VIIe. Water and acids	water	3.08	-1.79	-4.76	0.87	0.03
	formic acid	3.09	-0.06	-3.03	0.73	0.04
	acetic acid	1.86	-0.09	-2.56	1.01	0.25
	propionic acid	1.67	-0.35	-1.92	0.85	0.29
	butyric acid	1.52	-0.56	-1.58	1.15	0.37
	isobutyric acid	1.47	-0.57	-1.58	0.97	0.38
	3-methylbutanoic acid	1.34	-0.71	-1.26	1.22	0.55
	1-butanecarboxylic acid	1.33	-0.74	-1.19	1.28	0.47
	hexanoic acid	1.12	-0.85	-0.94	1.50	0.61
	n-heptanoic acid	1.02	-1.04	-0.68	1.62	0.84
	n-octanoic acid	1.13	-1.33	-0.22	1.37	1.12
	n-nonanoic acid	1.03	-1.21	-0.05	1.32	1.67
	benzoic acid	1.83	0.54	-0.29	2.21	-0.05
	m-phthalic acid	2.90	0.22	-0.98	4.24	0.38
Min VIIe		1.02	-1.79	-4.76	0.73	-0.05
Max VIIe		3.09	0.54	-0.05	4.24	1.67
Min VII		-0.44	-2.52	-4.76	-0.10	-1.49
Max VII		3.09	0.93	2.16	4.24	2.62

VIII. Amines and pyridines (100)

VIIia. Amines	ethylamine	0.02	-1.57	-0.81	-1.51	-1.14
	N-propyl amine	-0.15	-1.68	-0.49	-1.22	-1.11
	di-N-propylamine	-0.89	-1.80	0.19	-0.56	-0.59
	N-butylamine	-0.28	-1.75	-0.08	-1.22	-0.93
	isobutylamine	-0.36	-1.76	-0.30	-0.97	-0.93
	triethylamine	-1.27	-1.96	0.42	-0.78	-0.81
	tris-n-butylamine	-1.82	-2.14	1.42	0.44	0.40
	dibutyl amine	-1.11	-2.10	0.65	-0.28	-0.25
	N,N-di-isopropylamine	-0.87	-1.73	0.15	-0.57	-0.57
	tert-butylamine	-0.45	-1.63	-0.39	-1.12	-0.75
	diethylamine	-0.70	-1.58	-0.19	-1.07	-1.00
	N-methylbutylamine	-0.69	-1.73	-0.01	-0.75	-0.75
	hexylamine	-0.58	-1.98	0.19	-0.59	-0.51
	N,N-dimethylpropylamine	-1.03	-1.41	0.05	-0.98	-0.79
	dimethylamine	-0.26	-1.36	-0.91	-1.48	-1.24
	methylamine	0.31	-1.20	-1.24	-1.63	-1.34
	tripropylamine	-1.50	-1.81	0.83	-0.13	-0.13
	N-propyl-1-butanamine	-0.98	-1.92	0.40	-0.37	-0.37
	N,N-dimethylmethanamine	-0.83	-1.12	-0.60	-1.49	-1.11
	1,2-ethylenediamine	0.70	-2.18	0.58	-1.59	-1.45
	cyclohexyl amine	-0.50	-1.69	0.28	-0.67	-0.76
	N,N-dimethylcyclohexylamine	-1.18	-1.59	0.76	-0.34	-0.63
	N-methylcyclohexylamine	-0.77	-1.72	0.53	-0.29	-0.74
	propargylamine	0.98	-0.40	-0.50	-0.56	-1.25
	aniline	0.72	0.18	0.76	0.63	-1.57
	N-methylaniline	0.31	0.12	0.99	0.32	-1.26
	ethyl aniline	0.04	-0.07	1.11	0.37	-0.97
	p-chloroaniline	1.17	0.58	0.81	0.83	-1.18
	benzylamine	0.20	-0.16	0.84	0.06	-1.12
	o-toluidine	0.62	-0.02	0.78	0.69	-1.37
	para-toluidine	0.61	-0.10	0.73	0.73	-1.38
	para-anisidine	0.92	-0.09	0.81	0.75	-1.05
	N-methylformanilide	0.79	0.85	1.35	-0.36	0.25
	cyclopropylamine	0.05	-1.20	-0.31	-1.05	-1.39
	triallylamine	-0.62	-0.51	1.31	-0.12	-0.31
	N,N-dimethylbenzenamine	-0.36	0.38	1.21	-0.08	-0.94
	N,N-dimethylbenzylamine	-0.61	-0.12	1.20	0.20	-0.80
	N-methylbenzylamine	-0.14	-0.25	1.07	0.21	-1.05
	N-(tert-Butyl)benzylamine	-0.41	-0.65	1.64	0.52	-0.41
	N,N,N',N'-tetramethylmethylenediamine	-0.82	-1.67	1.23	-0.59	-0.86
	diallylamine	-0.16	-0.61	0.67	-0.45	-0.79
	2-chlorobenzenamine	1.00	0.58	0.78	1.06	-1.31
	p-bromophenylamine	0.91	0.19	1.28	0.57	-1.56
	2,2,2-trifluoroethyamine	1.75	0.24	-1.19	-0.86	1.11
	ammonia	0.73	-1.92	-2.49	-2.63	-0.86
	hydrazine	0.65	-1.07	-1.40	-0.79	-1.28
	ethylenimine	0.28	-0.80	-0.86	-1.42	-0.99
	piperidine	-0.53	-1.73	0.37	-0.99	-1.20
	N-methylpiperidine	-1.03	-1.38	0.28	-0.76	-0.97

	1-formylpiperidine	0.58	-0.23	0.94	-1.23	0.25
	n,n-dimethylpiperazine	-0.94	-0.95	0.77	-0.15	-0.79
	1,1,3,3-tetramethylguanidine	0.34	-1.17	1.99	-1.30	-0.84
	morpholine	0.00	-0.91	0.22	-0.92	-0.77
	4-methylmorpholine	-0.29	-0.90	0.38	-0.74	-0.59
	formyl morpholine	0.90	0.01	0.60	-1.15	0.47
	cyano morpholine	1.11	-0.48	0.90	-1.51	-0.17
	quinoline	0.23	0.18	1.85	0.05	-1.41
	pyrrole	0.74	-0.17	0.30	0.37	-2.10
	n-methyl pyrrole	-0.04	0.32	0.74	-0.76	-1.37
	pyrrolidine	-0.31	-1.35	-0.13	-1.04	-1.08
	2-pyrrolidone	1.74	-0.35	-0.18	-0.33	-0.36
	n-methylpyrrolidine	-0.83	-1.21	0.11	-1.02	-1.01
	1-methyl-2-pyrrolidinone	0.81	-0.10	0.85	-1.47	0.09
	1-ethyl-2-pyrrolidinone	0.57	-0.30	0.95	-1.21	0.25
	n-isopropyl-2-pyrrolidino	0.41	-0.43	1.05	-0.94	0.46
	N-cyclohexyl-2-pyrrolidone	0.05	-0.65	1.64	-0.36	0.77
	quinuclidine	-0.85	-1.26	0.49	-0.60	-0.88
	pyrimidine	1.17	-0.17	0.27	0.14	-1.93
	N-methyl-imidazole	1.18	-0.55	0.91	-1.14	-1.63
	1,3-dimethyl-2-imidazolidinone	0.83	-0.25	1.38	-1.39	-0.07
	N,N-diethylaminobenzene	-0.67	-0.16	1.56	0.22	-0.59
	N-methylpyridone	1.16	0.34	1.28	-1.20	-0.40
	aziridine, 1-phenyl-	-0.06	0.37	1.23	-0.03	-0.93
	Min VIIIa	-1.82	-2.18	-2.49	-2.63	-2.10
	Max VIIIa	1.75	0.85	1.99	1.06	1.11
VIIIb. Pyridines	pyridine	0.37	0.00	0.90	-1.08	-1.41
	2-picoline	0.09	-0.17	0.87	-0.89	-1.26
	3-Picoline	0.17	0.00	0.84	-0.87	-1.13
	4-methylpyridine	0.23	-0.08	0.99	-0.97	-1.23
	4-ethylpyridine	0.07	-0.14	1.08	-0.75	-0.96
	4-vinylpyridine	0.19	0.16	1.18	-0.30	-1.15
	3,4-dimethylpyridine	0.11	-0.09	1.15	-0.80	-1.07
	2,6-dimethylpyridine	-0.23	-0.30	1.08	-0.72	-1.20
	2,6-di-t-butylpyridine	-1.03	-1.04	2.04	0.33	-0.21
	2-butyl-pyridine	-0.33	-0.53	1.45	-0.35	-0.73
	2,4-lutidine	-0.02	-0.24	1.08	-0.74	-1.14
	2,4,6-trimethylpyridine	-0.33	-0.27	1.28	-0.63	-1.00
	3-iodopyridine	0.53	0.57	1.38	-0.13	-1.49
	2-bromopyridine	0.56	0.29	1.36	-0.48	-1.52
	3-bromopyridine	0.42	0.49	1.16	-0.30	-1.44
	2-chloropyridine	0.46	0.55	0.87	-0.75	-1.24
	3-chloropyridine	0.48	0.55	0.81	-0.48	-1.45
	3,5-dichloropyridine	0.44	0.83	0.72	0.14	-1.72
	2-fluoropyridine	1.07	0.58	0.41	-0.54	-0.52
	2,6-difluoropyridine	1.34	1.07	0.05	-0.40	0.19
	pentafluoropyridine	1.40	1.65	-1.23	2.01	0.63
	4-methoxypyridine	0.53	-0.03	1.25	-1.04	-0.77
	4-dimethylaminopyridine	0.61	-0.50	2.07	-1.22	-1.17
	2-cyanopyridine	1.33	0.63	1.26	-1.42	-0.68

4-cyanopyridine	0.81	1.00	0.89	-0.63	-0.65
2,2'-bipyridine	0.50	-0.36	2.35	-0.11	-1.16
pyridine-N-oxide	1.40	1.47	-0.65	1.27	-0.50
Min VIIIb	-1.03	-1.04	-1.23	-1.42	-1.72
Max VIIIb	1.40	1.65	2.35	2.01	0.63
Min VIII	-1.82	-2.18	-2.49	-2.63	-2.10
Max VIII	1.75	1.65	2.35	2.01	1.11

IX. Thiols, sulfides, sulfoxides and thio compounds (49)

IXa.Thiols	ethanethiol	-0.13	-0.27	-0.24	-0.95	-1.94
	n-propanethiol	-0.30	-0.44	-0.02	-0.80	-1.72
	isopropanethiol	-0.30	-0.34	-0.01	-0.79	-1.70
	1-butanethiol	-0.48	-0.45	0.11	-0.48	-1.34
	isobutanethiol	-0.47	-0.48	0.15	-0.56	-1.48
	tert-butanethiol	-0.47	-0.43	0.13	-0.64	-1.50
	n-pantanethiol	-0.59	-0.66	0.36	-0.35	-1.28
	isopantanethiol	-0.56	-0.56	0.37	-0.38	-1.21
	n-hexanethiol	-0.71	-0.75	0.55	-0.15	-1.07
	n-heptanethiol	-0.87	-0.85	0.76	0.03	-0.83
	n-octanethiol	-0.94	-0.91	0.93	0.23	-0.59
	n-nonanethiol	-1.07	-1.02	1.13	0.41	-0.39
	n-decanethiol	-1.15	-1.06	1.31	0.60	-0.11
	thiophenol	0.04	0.56	0.64	0.42	-1.62
	2-mercaptoethanol	1.47	-0.93	-0.70	0.93	-1.59
	allyl mercaptan	0.13	0.27	0.15	-0.80	-1.68
	Min IXa	-1.15	-1.06	-0.70	-0.95	-1.94
	Max IXa	1.47	0.56	1.31	0.93	-0.11
IXb. Sulfides	hydrogen sulfide	0.62	0.12	-1.49	-0.98	-2.19
	dimethyl sulfide	-0.30	-0.11	-0.12	-1.14	-1.90
	diethyl sulfide	-0.78	-0.42	0.26	-0.72	-1.70
	di-n-propyl sulfide	-0.96	-0.71	0.73	-0.39	-1.18
	diisopropyl sulfide	-1.00	-0.61	0.67	-0.29	-1.23
	methyl-n-propyl sulfide	-0.65	-0.51	0.38	-0.82	-1.56
	dibutyl sulfide	-1.22	-0.89	1.05	0.02	-0.78
	diisoamyl sulfide	-1.39	-1.09	1.36	0.31	-0.34
	trimethylene sulfide	-0.24	0.16	0.09	-0.92	-1.90
	pentamethylene sulfide	-0.69	-0.32	0.55	-0.54	-1.77
	methyl phenyl sulfide	-0.08	0.56	1.17	-0.02	-1.32
	dimethyl disulfide	-0.33	1.22	0.26	0.10	-1.70
	diethyl disulfide	-0.80	0.84	0.67	0.36	-1.42
	Min IXb	-1.39	-1.09	-1.49	-1.14	-2.19
	Max IXb	0.62	1.22	1.36	0.36	-0.34
IXc. Sulfoxides	dimethyl sulfoxide	1.34	0.29	0.68	-1.85	0.15
	diethyl sulfoxide	0.53	-0.22	0.94	-1.48	-0.03
	phenyl methyl sulfoxide	1.09	0.62	1.86	-0.83	0.22
	diphenyl sulfoxide	0.70	0.70	2.59	0.47	0.82
	di-n-butylsulfoxide	-0.17	-0.61	1.65	-0.59	0.79
	dibenzyl sulfoxide	0.66	0.65	3.03	0.58	1.26
	tetramethylene sulfoxide	0.83	0.07	0.97	-1.52	0.01
	dimethyl sulfate	1.42	1.94	-0.48	-0.87	2.59
	diethyl sulfite	1.21	0.54	0.82	-1.49	1.53

	ethyl benzenesulfonate	1.38	1.46	1.75	-0.57	1.89
	methyl methylthiomethyl sulfoxide(MMTS)	0.97	-0.57	1.84	-1.23	-0.82
	3-methyl sulfolane	1.19	1.07	0.61	-1.43	1.87
	methyldisulfanyl methane	-0.01	0.34	0.76	-0.45	-2.28
	Min IXc	-0.17	-0.61	-0.48	-1.85	-2.28
	Max IXc	1.42	1.94	3.03	0.58	2.59
IXd. Thio compounds	thiophene	0.21	0.47	0.79	-0.37	-1.68
	2-methylthiophene	0.17	0.26	1.02	-0.46	-1.64
	2,5-dimethylthiophene	-0.16	0.13	1.20	-0.31	-1.59
	tetrahydrothiophene	-0.51	-0.20	0.29	-0.84	-1.83
	methylthiopyrrolidinone	0.99	-0.43	1.89	-1.26	-0.87
	ethyl isothiocyanate	0.60	0.28	0.90	-1.19	-1.60
	thiodiglycol	1.78	-1.17	-0.30	1.57	-0.63
	Min IXd	-0.51	-1.17	-0.30	-1.26	-1.83
	Max IXd	1.78	0.47	1.89	1.57	-0.63
	Min IX	-1.39	-1.17	-1.49	-1.85	-2.28
	Max IX	1.78	1.94	3.03	1.57	2.59

X. Phosphorus compounds (12)

	trimethyl phosphate	1.00	0.81	-0.15	-0.93	2.57
	triethyl phosphate	0.53	0.25	0.69	-0.62	2.91
	tri-n-butyl phosphate	-0.38	0.03	1.56	0.84	4.28
	trimethyl phosphite	0.34	-0.53	0.36	-0.69	0.29
	triethyl phosphite	-0.25	-0.97	1.03	-0.11	0.62
	triphenylphosphite	0.39	0.28	3.91	2.67	2.43
	trimethyl-phosphane	-0.63	-0.95	0.00	-1.21	-1.55
	diethyl (chloromethyl)phosphonate	1.15	0.36	1.14	-1.16	2.32
	dichloromethyl-phosphonic acid diethyl ester	1.21	0.61	1.44	-0.97	2.29
	methylphosphonic acid bis(dimethylamide)	0.90	-1.25	2.11	-1.90	0.90
	phosphoric acid hexamethyltriamide	0.56	-1.23	2.30	-1.42	1.00
	phosphorothioic triamide, hexamethyl-	1.67	-0.85	3.82	-2.33	1.10
	Min X	-0.63	-1.25	-0.15	-2.33	-1.55
	Max X	1.67	0.81	3.91	2.67	4.28

XI. Miscellaneous (11)

	triethylphosphine oxide	0.36	-0.78	0.94	-1.56	1.14
	trimethylphosphine oxide	1.23	-0.06	0.30	-2.26	1.49
	trimethylamine n-oxide	0.70	0.83	0.16	-1.46	0.36
	1,1-dimethyltrimethylene oxide	-0.48	0.01	-0.90	-0.70	0.28
	methanesulfonic acid dimethylamide	0.95	-0.53	1.62	-1.89	-0.24
	tetraethyl sulfamide	0.81	-0.32	2.73	-0.87	1.89
	tetramethylsilane	-1.33	0.13	-1.39	0.00	0.41
	ethyl N,N,-dibutylcarbamate	-0.57	-1.03	1.69	0.16	1.77
	tris-cyanoethoxypropane	0.93	0.07	0.72	-1.20	1.17
	acetic anhydride	0.91	1.05	-0.81	-1.16	1.43
	tert-butyl hydroperoxide	0.56	-1.14	-1.06	0.61	-0.14
	Min XI	-1.33	-1.14	-1.39	-2.26	-0.24
	Max XI	1.23	1.05	2.73	0.61	1.89

NB: For first principal component (the sign inversion values were used)