

Molecule name	Polarizability exp	Polarizability calc	Deviation
((3-Methylbutoxy)methyl)benzene	22.05	22.25	-0.20
((4-tert-Butylphenoxy)methyl)oxirane	23.78	24.01	-0.23
((Chloromethoxy)methyl)benzene	16.61	16.82	-0.21
(-)-alpha-Pinene	15.53	15.58	-0.05
(-)-Carveol	18.53	18.75	-0.22
(+)-alpha-Thujene	17.53	17.41	0.12
(1-Bromoethyl)benzene	17.38	17.34	0.04
(1-Bromovinyl)benzene	17.41	17.07	0.34
(1-Methylvinyl)cyclopropane	11.09	10.90	0.19
(2-Bromoethyl)benzene	17.35	17.32	0.03
(2-Bromoethyl)cyclohexane	17.72	17.73	-0.01
(2-Chloro-1,1-dimethylethyl)benzene	19.56	19.82	-0.26
(2-Iodoethyl)benzene	19.66	19.36	0.30
(2-Methyl-1-propenyl)benzene	18.23	17.87	0.36
(2-Phenylethyl)trichlorosilane	23.24	23.22	0.02
(3-Bromopropyl)benzene	19.01	19.16	-0.15
(3-Chloropropyl)benzene	17.53	17.99	-0.46
(3-Chloropropyl)trichlorosilane	17.15	17.22	-0.07
(3-Chloropropyl)trimethoxysilane	18.44	18.48	-0.04
(3-Chloropropyl)trimethylsilane	17.63	17.57	0.06
(4-Bromophenoxy)trimethylsilane	23.21	23.17	0.04
(4-Chlorophenyl)trichlorosilane	21.82	21.46	0.36
(4-Methoxyphenyl)trimethylsilane	22.57	22.49	0.08
(4-Methylphenyl)trimethylsilane	21.73	21.81	-0.08
(5Z,8Z,11Z,14Z)-Eicosatetraenoic acid	37.91	37.87	0.04
(6Z)-Octadecenoic acid	34.81	34.44	0.37
(9Z)-Octadecenoic acid	34.21	34.44	-0.23
(Bromomethyl)chlorodimethylsilane	14.89	14.89	0.00
(Bromomethyl)cyclohexane	15.84	15.90	-0.06
(Bromomethyl)oxirane	9.62	9.25	0.37
(Bromomethyl)trimethylsilane	15.10	15.09	0.01
(Chloromethoxy)ethane	8.99	8.92	0.07
(Chloromethyl)benzene	14.29	14.32	-0.03
(Chloromethyl)cyclopropane	9.56	9.23	0.33
(Chloromethyl)trichlorosilane	13.52	13.53	-0.01
(Chloromethyl)trimethylsilane	13.93	13.88	0.05
(cis-2-Bromovinyl)benzene	17.31	17.16	0.15
(Dichloromethyl)trichlorosilane	15.60	15.48	0.12
(Diethylamino fluoro oxophosphorus) (bis(diethylamino) oxophosphorus) oxide	33.15	33.16	-0.01

(Diethylamino fluoro oxophosphorus) (bis(dimethylamino) oxophosphorus) oxide	25.93	25.88	0.05
(Diethylamino fluoro oxophosphorus) (diethylamino ethoxy oxophosphorus) oxide	28.60	28.68	-0.08
(Diethylamino fluoro thiophosphorus) (bis(diethylamino) oxophosphorus) oxide	36.11	36.11	0.00
(Diethylamino fluoro thiophosphorus) (diethylamino fluoro oxophosphorus) oxide	27.36	27.39	-0.03
(Diethylamino)acetonitrile	13.16	13.29	-0.13
(Diethylamino)trimethylsilane	18.76	18.67	0.09
(Dimethylamino)acetonitrile	9.54	9.65	-0.11
(E)-2-Undecenal	21.32	21.16	0.16
(Ethoxy fluoro oxophosphorus) (diethoxy oxophosphorus) oxide	20.19	20.14	0.05
(Ethoxymethyl)oxirane	10.83	10.52	0.31
(Ethylthio)benzene	17.53	17.55	-0.02
(Fluoromethyl)benzene	12.32	12.39	-0.07
(Iodomethyl)benzene	17.81	17.52	0.29
(Isopropylthio)benzene	19.41	19.38	0.03
(Methoxymethyl)oxirane	9.16	8.67	0.49
(Methylsulfonyl)ethene	9.57	9.42	0.15
(Methylthio)acetic acid	10.05	10.04	0.01
(Methylthio)ethene	9.31	9.15	0.16
(trans-1-Butenyl)benzene	18.29	17.85	0.44
(trans-2-Bromovinyl)benzene	17.62	17.16	0.46
(Trichloromethyl)oxirane	12.02	12.01	0.01
(Z) 9-Octadecen-1-ol	34.38	34.36	0.02
[1,1'-Bicyclopentyl]-2-one	17.48	17.58	-0.10
1-(1,1,2,2-Tetrafluoroethoxy)dodecane	27.79	27.51	0.28
1-(1,1,2,2-Tetrafluoroethoxy)octadecane	38.55	38.53	0.02
1-(1-Cyclohexen-1-yl)ethanone	14.69	14.74	-0.05
1-(1-Hydroxycyclohexyl)ethanone	15.26	15.33	-0.07
1-(2-Cyanoethyl)-3-(2-hydroxyethyl)-imidazolium chloride	20.24	19.98	0.26
1-(2-Cyanoethyl)-3-(2-propen-1-yl)-imidazolium chloride	21.19	21.13	0.06
1-(2-Cyanoethyl)-3-octylimidazolium 3- sulfobenzoate	44.23	44.50	-0.27
1-(2-Furanyl)-1-propanone	13.44	13.19	0.25
1-(2-Furanyl)-2-propanone	13.19	13.19	0.00
1-(2-Furyl)-2-ethyl-3-aminopropane	17.95	18.10	-0.15
1-(2-Furyl)-2-ethyl-3-methylaminopropane	19.85	19.93	-0.08
1-(2-Furyl)-2-ethyl-3-propanol	17.25	17.30	-0.05

1-(2-Furyl)-2-isopropyl-3-aminopropane	19.80	19.92	-0.12
1-(2-Furyl)-2-methyl-3-aminopropane	16.21	16.26	-0.05
1-(2-Furyl)-2-methyl-3-methylaminopropane	17.99	18.09	-0.10
1-(2-Furyl)-2-methyl-3-propanol	15.37	15.46	-0.09
1-(2-Furyl)-2-oxa-4-butanol	14.23	14.31	-0.08
1-(2-Furyl)-2-oxa-4-butyl acetate	19.15	19.39	-0.24
1-(2-Furyl)-2-oxa-4-pentanol	16.10	16.15	-0.05
1-(2-Furyl)-2-oxa-4-pentyl acetate	21.09	21.23	-0.14
1-(2-Furyl)-3-aminobutane	16.17	16.25	-0.08
1-(2-Furyl)-3-aminoheptane	21.53	21.76	-0.23
1-(2-Furyl)-3-aminohexane	19.76	19.92	-0.16
1-(2-Furyl)-3-aminononane	25.16	25.43	-0.27
1-(2-Furyl)-3-aminopentane	17.95	18.09	-0.14
1-(2-Furyl)-3-ethyl-1-penten-3-ol	21.10	20.89	0.21
1-(2-Furyl)-3-ethyl-3-pentanol	20.86	20.97	-0.11
1-(2-Furyl)-3-methyl-1-penten-3-ol	19.15	19.05	0.10
1-(2-Furyl)-3-methyl-3-pentanol	18.96	19.13	-0.17
1-(2-Furyl)-3-methylaminobutane	18.00	18.08	-0.08
1-(2-Furyl)-3-methylaminopentane	19.74	19.92	-0.18
1-(2-Furyl)-3-propanol	13.77	13.64	0.13
1-(2-Hydroxy-4-methylphenyl)ethanone	17.29	16.97	0.32
1-(2-Hydroxy-5-methylphenyl)-1-propanone	19.10	18.81	0.29
1-(2-Hydroxyethyl)-3-methylimidazolium perfluoropentanoate	24.70	24.33	0.37
1-(2-Methylphenyl)ethanone	15.95	16.27	-0.32
1-(2-Pyridinyl)ethanone	13.56	13.52	0.04
1-(2-Tetrahydrofuryl)-3-aminobutane	16.70	16.69	0.01
1-(2-Tetrahydrofuryl)-3-butanone	15.31	15.46	-0.15
1-(3-Cyanopropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl) amide	29.59	29.67	-0.08
1-(3-Cyanopropyl)-3-methylimidazolium dicyanamide	22.58	22.75	-0.17
1-(3-Cyanopropyl)-3-methylimidazolium tetrafluoroborate	18.58	18.88	-0.30
1-(3-Cyanopropyl)-pyridinium bis(trifluoromethylsulfonyl) amide	30.02	30.14	-0.12
1-(3-Cyanopropyl)-pyridinium dicyanamide	22.89	23.23	-0.34
1(3H)-Isobenzofuranone	14.25	14.17	0.08
1-(3-Methylphenyl)ethanone	16.24	16.27	-0.03
1-(4-Isopropylphenyl)ethanone	20.16	19.92	0.24
1-(4-Methylphenyl)-1-propanone	18.22	18.10	0.12
1-(4-Methylphenyl)ethanol	17.10	16.72	0.38
1-(Bromomethoxy)-2-methylbutane	16.21	16.05	0.16

1-(Bromomethoxy)-2-methylpropane	14.13	14.21	-0.08
1-(Bromomethoxy)-3-methylbutane	16.02	16.05	-0.03
1-(Bromomethyl)-2-methylbenzene	17.50	17.39	0.11
1-(Bromomethyl)-3-methylbenzene	17.45	17.39	0.06
1-(Chloromethoxy)propane	10.85	10.75	0.10
1-(Chloromethyl)-2-fluorobenzene	14.21	14.28	-0.07
1-(Chloromethyl)-2-methylbenzene	16.48	16.23	0.25
1-(Chloromethyl)-3-methylbenzene	16.30	16.23	0.07
1-(Chloromethyl)-4-fluorobenzene	14.19	14.28	-0.09
1-(Chloromethyl)-4-methylbenzene	16.59	16.23	0.36
1-(Chloromethyl)naphthalene	21.30	21.44	-0.14
1-(Dimethylamino)-2-propanol	12.35	12.13	0.22
1,1,1,2,3,3,3-Heptachloropropane	19.88	19.91	-0.03
1,1,1,2-Tetrachloroacetone	13.99	14.20	-0.21
1,1,1,2-Tetrachloroethane	12.32	12.26	0.06
1,1,1,2-Tetrachloropropane	14.07	14.08	-0.01
1,1,1,3,3,3-Hexafluoro-2-methoxypropane	9.23	9.07	0.16
1,1,1,3,5,5,5-Heptamethyltrisiloxane	25.04	25.07	-0.03
1,1,1,3,5,7,7,7-Octamethyltetrasiloxane	30.71	30.73	-0.02
1,1,1,3-Tetrachloropropane	14.18	14.09	0.09
1,1,1-Bromodichloroethane	11.50	11.47	0.03
1,1,1-Chlorodifluoro-2-iodoethane	11.46	11.59	-0.13
1,1,1-Chlorodifluoro-4-iodobutane	15.29	15.27	0.02
1,1,1-Tributoxypropane	30.08	30.07	0.01
1,1,1-Trichloroacetone	12.29	12.30	-0.01
1,1,1-Trichlorotrifluoroethane	10.41	10.46	-0.05
1,1,1-Triethoxyethane	17.54	17.22	0.32
1,1,1-Triethoxypropane	19.13	19.06	0.07
1,1,1-Trifluoro-2-iodoethane	9.49	9.74	-0.25
1,1,1-Trifluoro-2-propanol	6.96	7.03	-0.07
1,1,1-Trifluoroethane	4.40	4.63	-0.23
1,1,1-Trihexoxypropane	40.95	41.08	-0.13
1,1,1-Trimethoxyethane	11.85	11.68	0.17
1,1,1-Trioctyloxypropane	51.91	52.09	-0.18
1,1,1-Tripropoxypropane	24.28	24.56	-0.28
1,1,2,2,3-Pentachloropropane	15.70	15.90	-0.20
1,1,2,2-Tetrabromobutane	20.25	20.43	-0.18
1,1,2,2-Tetrabromoethane	16.55	16.63	-0.08
1,1,2,2-Tetrachloro-1,2-difluoroethane	12.25	12.20	0.05
1,1,2,2-Tetrachloro-1-fluoroethane	12.50	12.19	0.31
1,1,2,2-Tetrachloroethane	12.14	12.18	-0.04
1,1,2,2-Tetrachlorohexane	19.53	19.51	0.02

1,1,2,2-Tetra-t-butylethane	33.80	33.82	-0.02
1,1,2,3,3-Pentachloro-1-propene	16.11	15.90	0.21
1,1,2,3-Tetrachloropropane	14.10	13.97	0.13
1,1,2-Tribromobutane	17.37	17.33	0.04
1,1,2-Tribromoethane	13.68	13.64	0.04
1,1,2-Tribromopropane	15.71	15.50	0.21
1,1,2-Trichloroethane	10.27	10.25	0.02
1,1,2-Trimethylcyclohexane	16.50	16.49	0.01
1,1,2-Trimethylcyclopentane	14.69	14.66	0.03
1,1,2-Trimethylcyclopropane	11.37	10.99	0.38
1,1,3,3-Tetramethoxypropane	16.11	16.20	-0.09
1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane	35.23	35.16	0.07
1,1,3,3-Tetramethylcyclopentane	16.69	16.50	0.19
1,1,3,3-Tetramethyldisiloxane	15.93	15.95	-0.02
1,1,3,3-Tetramethylguanidinium butanoate	22.29	22.25	0.04
1,1,3,3-Tetramethylguanidinium heptanoate	28.00	27.76	0.24
1,1,3,3-Tetramethylguanidinium hexanoate	25.66	25.92	-0.26
1,1,3,3-Tetramethylguanidinium octanoate	29.48	29.59	-0.11
1,1,3,3-Tetramethylguanidinium pentanoate	24.12	24.09	0.03
1,1,3,5,7,9-Hexaethoxydecane	44.70	44.67	0.03
1,1,3,5,7-Pentaethoxyoctane	36.96	36.79	0.17
1,1,3,5-Tetraethoxy-5-methylhexane	30.92	30.98	-0.06
1,1,3-Trichloropropane	12.07	12.09	-0.02
1,1,3-Trimethylcyclopentane	14.87	14.66	0.21
1,10-Decanediol bis(perfluorobutyrate)	36.34	36.10	0.24
1,10-Decanedithiol	25.30	25.28	0.02
1,10-Dichlorodecane	23.00	23.01	-0.01
1,10-Undecadiyne	19.41	19.42	-0.01
1,11-Undecanedithiol	27.11	27.12	-0.01
1,13-Tridecanedioic acid	25.92	25.98	-0.06
1,14-Tetradecanedioic acid	27.76	27.81	-0.05
1,1-Bis(butylthio)ethane	25.50	25.46	0.04
1,1-Bis(ethoxycarbonyl)-2-methylcyclopentane	23.21	23.39	-0.18
1,1-Bis(ethylthio)-2-butyne	20.93	21.19	-0.26
1,1-Bis(ethylthio)ethane	18.13	18.12	0.01
1,1-Bis(ethylthio)propane	21.69	21.79	-0.10
1,1-Bis(isobutylthio)ethane	25.39	25.43	-0.04
1,1-Bis(isopropylthio)ethane	21.81	21.78	0.03
1,1-Bis(methoxycarbonyl)cyclohexane	19.49	19.71	-0.22
1,1-Bis(methylthio)-cyclohexane	20.83	20.89	-0.06
1,1-Bis(methylthio)propane	16.42	16.11	0.31
1,1-Bis(propylthio)ethane	21.61	21.79	-0.18

1,1-Cyclohexanedithiol	17.13	17.19	-0.06
1,1-Di(2-chloroethoxy)ethane	17.07	16.94	0.13
1,1-Dibromo-1-butene	13.98	14.12	-0.14
1,1-Dibromo-1-heptene	19.76	19.63	0.13
1,1-Dibromo-1-hexene	17.73	17.79	-0.06
1,1-Dibromo-1-octene	21.71	21.46	0.25
1,1-Dibromo-1-pentene	15.88	15.96	-0.08
1,1-Dibromo-1-propene	12.28	12.28	0.00
1,1-Dibromobutane	14.08	14.25	-0.17
1,1-Dibromoethane	10.64	10.58	0.06
1,1-Dibromopropane	12.08	12.41	-0.33
1,1-Dibutylhydrazine	18.44	18.41	0.03
1,1-Dichloro-1,3-butadiene	12.17	11.83	0.34
1,1-Dichloro-1-fluoroethane	8.19	8.36	-0.17
1,1-Dichloro-2,2-difluoroethane	8.02	8.30	-0.28
1,1-Dichloro-2-fluoropropene	9.92	10.08	-0.16
1,1-Dichloro-2-methylpropane	11.81	12.00	-0.19
1,1-Dichloro-3,3-dimethylbutane	15.75	15.68	0.07
1,1-Dichloro-3,3-dimethylpentane	17.45	17.52	-0.07
1,1-Dichlorobutane	12.11	12.02	0.09
1,1-Dichlorocyclohexane	14.92	14.83	0.09
1,1-Dichloroethane	8.38	8.35	0.03
1,1-Dichloropropane	10.20	10.18	0.02
1,1-Dichloropropene	9.83	10.12	-0.29
1,1-Diethoxycyclohexane	19.29	19.59	-0.30
1,1-Diethoxycyclopentane	17.69	17.75	-0.06
1,1-Diethoxyethane	13.25	13.14	0.11
1,1-Diethoxypentane	18.69	18.64	0.05
1,1-Diethoxypropane	15.14	14.97	0.17
1,1-Diethylhydrazine	11.08	11.07	0.01
1,1-Difluoro-1,2,2-trichloroethane	10.28	10.32	-0.04
1,1-Difluoro-1-ethoxy-2-iodoethane	14.07	14.31	-0.24
1,1-Dimethoxyhexadecane	34.92	35.14	-0.22
1,1-Dimethylbutyl acetate	15.99	16.20	-0.21
1,1-Dimethylcyclohexane	14.69	14.67	0.02
1,1-Dimethylcyclopentane	12.96	12.84	0.12
1,1-Dimethylcyclopropane	9.45	9.17	0.28
1,1-Dimethylhydrazine	7.42	7.43	-0.01
1,1-Dimethylindane	18.98	18.98	0.00
1,1-Dimethylpropargylamine	10.63	10.55	0.08
1,1-Dipentylhydrazine	22.10	22.08	0.02
1,1-Diphenylbutane	27.41	27.64	-0.23

1,1-Diphenylethane	23.90	23.97	-0.07
1,1-Diphenylethylene	24.16	23.89	0.27
1,1-Dipropoxyethane	16.80	16.81	-0.01
1,1-Dipropylhydrazine	14.77	14.74	0.03
1,1-Ethanediol diacetate	13.08	13.18	-0.10
1,1-Propanedithiol	14.16	14.25	-0.09
1,2,2,3-Tetrabromobutane	20.38	20.53	-0.15
1,2,2,3-Tetrachloropropane	13.99	13.98	0.01
1,2,2-Tribromobutane	17.62	17.45	0.17
1,2,2-Tribromopropane	15.82	15.61	0.21
1,2,2-Trichloropropane	12.17	12.07	0.10
1,2,2-Trimethylpropylacetate	16.19	16.22	-0.03
1,2,2-Tris(butylthio)-propane	37.80	37.89	-0.09
1,2,2-Tris(isobutylthio)-propane	37.65	37.84	-0.19
1,2,2-Tris(isopropylthio)-propane	32.20	32.37	-0.17
1,2,2-Tris(propylthio)-propane	32.37	32.39	-0.02
1,2,3,4,5,6,7,8-Octahydroanthracene	23.78	23.78	0.00
1,2,3,4-Tetrachloro-5,5-dimethoxy-1,3-cyclopentadiene	21.47	21.70	-0.23
1,2,3,4-Tetrachlorobutadiene	15.87	15.65	0.22
1,2,3,4-Tetrafluorobenzene	10.07	10.35	-0.28
1,2,3,4-Tetrahydro-1,1,6-trimethylnaphthalene	22.79	22.72	0.07
1,2,3,4-Tetrahydro-1,5-dimethylnaphthalene	20.72	20.87	-0.15
1,2,3,4-Tetrahydro-6-methylnaphthalene	18.94	19.05	-0.11
1,2,3,4-Tetrahydroisoquinoline	16.20	16.65	-0.45
1,2,3,4-Tetrahydronaphthalene	17.08	17.15	-0.07
1,2,3,4-Tetrahydroquinoline	17.20	16.95	0.25
1,2,3,4-Tetramethylcyclohexane	18.29	18.29	0.00
1,2,3,5-Tetramethylbenzene	17.96	18.14	-0.18
1,2,3-Propanetriol	8.14	8.04	0.10
1,2,3-Tribromobutane	17.45	17.43	0.02
1,2,3-Tribromopropane	15.44	15.58	-0.14
1,2,3-Trichloro-1,1,2,3,3-pentafluoropropane	12.21	12.26	-0.05
1,2,3-Trichloropropane	12.06	12.05	0.01
1,2,3-Trichloropropene	12.07	11.99	0.08
1,2,3-Trimethylindene	20.64	20.78	-0.14
1,2,4,5-Tetrafluorobenzene	10.29	10.35	-0.06
1,2,4,5-Tetramethylbenzene	18.00	18.14	-0.14
1,2,4a,5,8,8a-Hexahydro-4,7-dimethyl-1-isopropylnaphthalene	26.07	26.52	-0.45
1,2,4-Tribromobutane	17.43	17.41	0.02
1,2,4-Trichlorobenzene	16.21	16.24	-0.03

1,2,4-Triethylbenzene	21.74	21.74	0.00
1,2,4-Trifluorobenzene	10.42	10.39	0.03
1,2,4-Triisopropylbenzene	27.30	27.20	0.10
1,2,4-Trimethyl-5-hexadecylbenzene	45.57	45.67	-0.10
1,2,4-Trimethyl-5-hexadecylcyclohexane	45.69	45.82	-0.13
1,2,4-Trimethylbenzene	16.13	16.23	-0.10
1,2,5,6-Tetrahydropyridine	10.27	10.43	-0.16
1,2,5-Trimethylpyrrole	13.87	13.89	-0.02
1,2-Benzopyran	16.01	15.92	0.09
1,2-Bis(1,1,2,2-tetrafluoroethoxy)ethane	14.00	13.80	0.20
1,2-Bis(2-chloroethoxy)ethane	16.97	17.01	-0.04
1,2-Bis(dimethylamino)ethane	15.07	14.95	0.12
1,2-Bis(dipentylborinoxy)ethane	46.03	46.02	0.01
1,2-Bis(tributylsilyl)acetylene	54.73	54.79	-0.06
1,2-Bis(triethylsilyl)ethane	33.93	34.02	-0.09
1,2-Bis(trimethylsilyl)acetylene	21.87	21.90	-0.03
1,2-Butadiene	8.04	8.17	-0.13
1,2-Butanediol	9.35	9.31	0.04
1,2-Cycloheptanedione	13.16	13.06	0.10
1,2-Cyclohexanedione	11.68	11.23	0.45
1,2-Diaminobenzene	13.80	13.74	0.06
1,2-Dibromo-1,1-difluoroethane	10.63	10.64	-0.01
1,2-Dibromo-1,3,4,4-tetrachlorobutane	21.89	21.94	-0.05
1,2-Dibromo-2-methylpropane	14.41	14.39	0.02
1,2-Dibromo-4,4-dimethylhexane	21.60	21.68	-0.08
1,2-Dibromo-4,4-dimethylpentane	19.90	19.84	0.06
1,2-Dibromobenzene	16.46	16.53	-0.07
1,2-Dibromoethane	10.70	10.66	0.04
1,2-Dibromoheptane	19.89	19.85	0.04
1,2-Dibromohexane	18.11	18.02	0.09
1,2-Dibromopentane	16.32	16.18	0.14
1,2-Dibromopropane	12.59	12.51	0.08
1,2-Dibromotetrafluoroethane	10.60	10.63	-0.03
1,2-Dibutoxyethane	20.63	20.54	0.09
1,2-Dichloro-1,1-difluoroethane	8.38	8.39	-0.01
1,2-Dichloro-1,2-difluoroethane	8.38	8.41	-0.03
1,2-Dichloro-1,3-butadiene	11.88	11.80	0.08
1,2-Dichloro-1-fluoroethane	8.37	8.37	0.00
1,2-Dichloro-2-methylpropane	12.07	12.04	0.03
1,2-Dichloro-3,3,4,4,5,5-hexafluorocyclopentene	13.20	13.45	-0.25
1,2-Dichloro-3,4-dimethylpentane	17.52	17.45	0.07
1,2-Dichloro-4-(trichloromethyl)benzene	22.18	22.08	0.10



1,2-Dichloro-4,4-dimethylhexane	19.22	19.31	-0.09
1,2-Dichlorobenzene	14.25	14.33	-0.08
1,2-Dichlorobutane	12.05	11.98	0.07
1,2-Dichlorohexafluoropropane	10.52	10.41	0.11
1,2-Dichloronaphthalene	21.24	21.45	-0.21
1,2-Dichloropentane	13.78	13.81	-0.03
1,2-Dichloropropane	10.20	10.14	0.06
1,2-Diethoxybenzene	19.51	19.38	0.13
1,2-Diethylbenzene	17.89	18.00	-0.11
1,2-Diethylhydrazine	11.10	11.01	0.09
1,2-Diethylpyridinium ethylsulfate	25.56	25.54	0.02
1,2-Difluorobenzene	10.38	10.43	-0.05
1,2-Dihydronaphthalene	17.26	17.07	0.19
1,2-Diiodobenzene	20.29	20.48	-0.19
1,2-Diisobutylhydrazine	18.37	18.32	0.05
1,2-Diisopropylbenzene	21.60	21.64	-0.04
1,2-Diisopropylhydrazine	14.68	14.63	0.05
1,2-Dimethoxy-4-allylbenzene	21.12	21.14	-0.02
1,2-Dimethyl-3-nitrobenzene	16.59	16.97	-0.38
1,2-Dimethyl-5-propylpyrrole	17.66	17.56	0.10
1,2-Dimethyl-5-propylpyrrolidine	17.84	17.99	-0.15
1,2-Dimethylbenzene	14.20	14.33	-0.13
1,2-Dimethylcyclohexene	14.61	14.66	-0.05
1,2-Dimethylcyclopentene	12.79	12.82	-0.03
1,2-Dimethylenecyclohexane	14.36	14.49	-0.13
1,2-Dimethylhydrazine	7.30	7.37	-0.07
1,2-Dimethylnaphthalene	21.28	21.45	-0.17
1,2-Dimethylpiperidine	14.34	14.35	-0.01
1,2-Dimethylpropylamine	11.29	11.34	-0.05
1,2-Dinitroethane	8.71	9.07	-0.36
1,2-Diphenylbutane	27.68	27.64	0.04
1,2-Dipiperidinoethane	24.36	24.20	0.16
1,2-Dipropoxyethane	16.95	16.87	0.08
1,2-Dis(trimethylsilyl)-ethylene	23.19	23.01	0.18
1,2-Epoxy-4-(epoxyethyl)cyclohexane	14.36	14.32	0.04
1,2-Ethanediol	5.73	5.64	0.09
1,2-Ethanediol dinitrate	10.49	10.56	-0.07
1,2-Ethanedithiol	10.72	10.60	0.12
1,2-Oxathiane 2,2-dioxide	11.19	11.12	0.07
1,2-Pentadiene	9.89	10.01	-0.12
1,2-Pentenediol	11.18	11.15	0.03
1,2-Propanediol	7.56	7.48	0.08

1,2-Propanediol diacetate	15.09	15.09	0.00
1,2-Propanediolsulfite	9.79	9.99	-0.20
1,3,4,4-Tetrachloro-1-butene	15.76	15.69	0.07
1,3,4,5,6,6-Hexachloro-1-hexene	23.06	23.13	-0.07
1,3,5-Cycloheptatriene	12.80	12.61	0.19
1,3,5-Cyclooctatriene	14.21	14.44	-0.23
1,3,5-Tributylborazine	31.55	31.66	-0.11
1,3,5-Triethylbenzene	21.81	21.74	0.07
1,3,5-Triethylborazine	20.80	20.64	0.16
1,3,5-Trifluorobenzene	10.25	10.39	-0.14
1,3,5-Triisopropylbenzene	27.32	27.20	0.12
1,3,5-Trimethyl-1H-pyrazole	12.88	13.01	-0.13
1,3,5-Trimethyladamantane	22.53	22.12	0.41
1,3,5-Trimethylbenzene	16.25	16.23	0.02
1,3,5-Trisilacyclohexane	17.32	17.22	0.10
1,3,6-Tricyanohexane	17.02	17.10	-0.08
1,3-Benzodioxole	12.79	12.93	-0.14
1,3-Bis(1-methyl-4-piperidyl)propane	29.98	29.68	0.30
1,3-Bis(1-methylethenyl)benzene	21.83	21.48	0.35
1,3-Bis(bromomethyl)tetramethyldisiloxane	25.53	25.55	-0.02
1,3-Bis(chloromethyl)tetramethyldisiloxane	23.11	23.11	0.00
1,3-Bis(dibutoxyboryl)propane	41.51	41.55	-0.04
1,3-Bis(dichloroboryl)propane	17.49	17.54	-0.05
1,3-Bis(dichloromethyl)tetramethyldisiloxane	26.98	27.03	-0.05
1,3-Bis(dimethoxyboryl)propane	19.41	19.48	-0.07
1,3-Bis(dimethylamino)-2-propanol	17.45	17.35	0.10
1,3-Bis(trifluoromethyl)benzene	14.64	14.55	0.09
1,3-Bis(trimethylsiloxy)benzene	29.88	29.80	0.08
1,3-Butanediol dinitrate	14.09	14.23	-0.14
1,3-Butanediolsulfite	12.01	11.83	0.18
1,3-Butyleneglycol	9.37	9.31	0.06
1,3-Cycloheptadiene	12.60	12.69	-0.09
1,3-Cyclohexadiene	10.65	10.85	-0.20
1,3-Cyclohexanedione	11.16	11.23	-0.07
1,3-Di(4-methylpentyl)-1,3-diphospha-2,4-dithiacyclobutane 1,3-dithioxide	42.40	42.56	-0.16
1,3-Diacetin	15.59	15.65	-0.06
1,3-Diaminobenzene	13.46	13.74	-0.28
1,3-Dibromo-1,1-dichloropropane	16.34	16.37	-0.03
1,3-Dibromo-2,2-dimethylpropane	16.22	16.15	0.07
1,3-Dibromo-2-propanol	12.87	13.05	-0.18
1,3-Dibromobenzene	16.57	16.53	0.04

1,3-Dibromobutane	14.15	14.35	-0.20
1,3-Dibromopropane	12.36	12.49	-0.13
1,3-Dibromopropyne	11.74	11.75	-0.01
1,3-Dichloro-2-propanol	10.83	10.72	0.11
1,3-Dichloro-2-propanol nitrate	12.91	13.18	-0.27
1,3-Dichloroacetone	10.19	10.27	-0.08
1,3-Dichlorobenzene	14.32	14.33	-0.01
1,3-Dichlorobutane	12.00	11.98	0.02
1,3-Dichloropropane	10.12	10.16	-0.04
1,3-Dichloro-trans-2-butene	11.96	11.96	0.00
1,3-Diethylbenzene	18.05	18.00	0.05
1,3-Diethylimidazolium bis(trifluoromethylsulfonyl) amide	27.86	27.90	-0.04
1,3-Difluoro-2-propanol	6.99	6.85	0.14
1,3-Difluorobenzene	10.25	10.43	-0.18
1,3-Difluoropropane	6.24	6.29	-0.05
1,3-Dihexyl-1,3-diphospha-2,4-dithiacyclobutane 1,3-dithioxide	42.59	42.59	0.00
1,3-Diiodohexafluoropropane	16.72	16.66	0.06
1,3-Diiodopropane	16.48	16.57	-0.09
1,3-Diisopropylbenzene	21.66	21.64	0.02
1,3-Dimethoxy-1-ethoxy-5-methyl-4-hexene	22.69	22.91	-0.22
1,3-Dimethoxybenzene	15.90	15.68	0.22
1,3-Dimethyl-1H-pyrazole	11.19	11.18	0.01
1,3-Dimethyl-2-oxo-hexahydro-pyrimidine	13.81	13.67	0.14
1,3-Dimethyladamantane	20.44	20.28	0.16
1,3-Dimethylbenzene	14.33	14.33	0.00
1,3-Dimethylcyclohexene	14.66	14.62	0.04
1,3-Dimethylimidazolium bis(trifluoromethylsulfonyl) amide	24.01	24.26	-0.25
1,3-Dimethylimidazolium methosulfate	17.75	17.76	-0.01
1,3-Dimethylnaphthalene	21.28	21.45	-0.17
1,3-Dinitropropane	10.87	10.90	-0.03
1,3-Dioxane	8.53	8.59	-0.06
1,3-Dioxolan-2-one	6.61	6.78	-0.17
1,3-Dioxolane	6.68	6.76	-0.08
1,3-Dipentyl-1,3-diphospha-2,4-dithiacyclobutane 1,3-dithioxide	39.05	38.92	0.13
1,3-Diphenyl-1-butene	27.87	27.57	0.30
1,3-Diphenylpropane	25.57	25.83	-0.26
1,3-Dipropylimidazolium bis(trifluoromethylsulfonyl) amide	31.60	31.57	0.03
1,3-Dithiolane	11.40	11.71	-0.31

1,3-Divinyl-1,1,3,3-tetramethyldisiloxane	22.69	22.73	-0.04
1,3-Pentadiyne	8.52	8.62	-0.10
1,3-Propanediamine	9.11	9.07	0.04
1,3-Propanediol	7.54	7.47	0.07
1,3-Propanediol diacetate	14.99	15.08	-0.09
1,4-Bis(3-aminopropoxy)butane	23.19	23.26	-0.07
1,4-Bis(acetoxy)-2-butyne	16.22	16.32	-0.10
1,4-Bis(butanoyloxy)-2-butyne	23.55	23.67	-0.12
1,4-Bis(dichloroboryl)butane	19.34	19.38	-0.04
1,4-Bis(diethoxyboryl)butane	28.98	28.71	0.27
1,4-Bis(formoxy)-2-butyne	12.60	12.76	-0.16
1,4-Bis(heptanoyloxy)-2-butyne	34.62	34.68	-0.06
1,4-Bis(hexanoyloxy)-2-butyne	30.92	31.01	-0.09
1,4-Bis(propanoyloxy)-2-butyne	19.86	19.99	-0.13
1,4-Bis(valeroyloxy)-2-butyne	27.23	27.34	-0.11
1,4-Butanediol diacetate	16.85	16.92	-0.07
1,4-Butanediol diglycidyl ether	20.00	20.19	-0.19
1,4-Butanediol dimethacrylate	23.79	24.07	-0.28
1,4-Butanedithiol	14.32	14.27	0.05
1,4-Cyclohexadiene	10.51	10.85	-0.34
1,4-Diaminobenzene	13.80	13.74	0.06
1,4-Dibromo-2-butyne	14.04	13.73	0.31
1,4-Dibromobutane	14.22	14.33	-0.11
1,4-Dibromopentane	16.25	16.18	0.07
1,4-Dichloro-2-butyne	11.51	11.40	0.11
1,4-Dichlorobenzene	14.39	14.33	0.06
1,4-Dichlorobutane	11.99	12.00	-0.01
1,4-Dichloronaphthalene	21.19	21.45	-0.26
1,4-Diethylbenzene	18.05	18.00	0.05
1,4-Difluorobenzene	10.23	10.43	-0.20
1,4-Difluorobutane	8.07	8.13	-0.06
1,4-Difluorooctachlorobutane	23.32	23.51	-0.19
1,4-Dihydronaphthalene	16.75	17.07	-0.32
1,4-Dihydroxybenzene	11.73	11.92	-0.19
1,4-Diiodobutane	18.33	18.40	-0.07
1,4-Diisopropylbenzene	21.70	21.64	0.06
1,4-Dimethyl-2-nitrobenzene	16.64	16.97	-0.33
1,4-Dimethyl-2-propylpyrrolidine	17.91	18.00	-0.09
1,4-Dimethylbenzene	14.27	14.33	-0.06
1,4-Dimethylnaphthalene	21.20	21.45	-0.25
1,4-Dimethylpiperazine	14.07	14.07	0.00
1,4-Dioxane	8.59	8.68	-0.09

1,4-Dioxatetralin	14.54	14.86	-0.32
1,4-Divinylbenzene	18.16	17.75	0.41
1,4-Oxathiane	11.01	11.15	-0.14
1,4-Pentadien-3-ol	10.22	10.34	-0.12
1,4-Pentadiene	9.66	9.78	-0.12
1,4-Pentanediol	11.12	11.15	-0.03
1,4-Piperazinedipropanamine	24.07	24.10	-0.03
1,5-Bis(diethoxyboryl)pentane	30.57	30.54	0.03
1,5-Diazabicyclo[4.3.0]non-5-ene	14.87	14.77	0.10
1,5-Dibromoheptane	19.78	19.85	-0.07
1,5-Dibromopentane	16.11	16.16	-0.05
1,5-Dibromoundecane	27.53	27.19	0.34
1,5-Dichloropentane	13.83	13.83	0.00
1,5-Difluoropentane	9.93	9.96	-0.03
1,5-Diiodopentane	20.22	20.24	-0.02
1,5-Dimethylcyclopentene	12.70	12.78	-0.08
1,5-Hexadiene	11.58	11.61	-0.03
1,5-Hexadiyne	10.10	10.24	-0.14
1,5-Pentanediamine	12.78	12.74	0.04
1,5-Pentanediol	11.18	11.14	0.04
1,5-Pentanediol diacetate	18.57	18.75	-0.18
1,5-Pentanedithiol	16.15	16.11	0.04
1,6-Bis(diethoxyboryl)hexane	32.43	32.38	0.05
1,6-Dibromohexane	17.91	18.00	-0.09
1,6-Dichlorohexane	15.64	15.67	-0.03
1,6-Difluorohexane	11.75	11.80	-0.05
1,6-Diiodohexane	22.03	22.07	-0.04
1,6-Dimethyl-4-isopropyl-naphthalene	27.01	27.01	0.00
1,6-Dimethylnaphthalene	21.61	21.45	0.16
1,6-Heptadiyne	12.05	12.08	-0.03
1,6-Hexamethylene diisocyanate	17.29	17.47	-0.18
1,6-Hexanedioic acid	13.07	13.13	-0.06
1,6-Hexanediol bis(6-H-perfluoroheptanoate)	40.34	40.36	-0.02
1,6-Hexanediol bis(perfluorobutyrate)	28.95	28.75	0.20
1,6-Hexanediol bis(perfluorooctanoate)	44.61	44.64	-0.03
1,6-Hexanedithiol	17.96	17.94	0.02
1,7-Dibromo-3,3-dichloroheptane	23.61	23.65	-0.04
1,7-Dibromoheptane	19.76	19.83	-0.07
1,7-Dichloroheptane	17.52	17.50	0.02
1,7-Dichloronaphthalene	21.45	21.45	0.00
1,7-Dimethylnaphthalene	21.18	21.45	-0.27
1,7-Heptanediol	14.77	14.81	-0.04

1,7-Heptanedithiol	19.57	19.78	-0.21
1,7-Octadiene	15.20	15.29	-0.09
1,7-Octadiyne	13.90	13.91	-0.01
1,8-Cineole	18.02	18.12	-0.10
1,8-Diaminonaphthalene	21.10	20.86	0.24
1,8-Dibromooctane	21.62	21.67	-0.05
1,8-Dichloronaphthalene	21.33	21.45	-0.12
1,8-Dichlorooctane	19.30	19.34	-0.04
1,8-Nonadiene	16.94	17.12	-0.18
1,8-Nonadiyne	15.67	15.75	-0.08
1,8-Octanedithiol	21.65	21.61	0.04
1,9-Decadiene	18.97	18.96	0.01
1,9-Dichlorononane	20.99	21.17	-0.18
1,9-Nonanedithiol	23.34	23.45	-0.11
1-[(2-Aminoethyl)amino]-2-propanol	13.38	13.28	0.10
10,11-Dipropyleicosane	48.35	48.54	-0.19
10-Chloro-1-decanol	21.64	21.66	-0.02
10-Undecen-1-ol	21.35	21.47	-0.12
10-Undecenoic acid	21.58	21.55	0.03
10-Undecenoyl chloride	23.05	23.08	-0.03
11,12-Dipropyldocosane	52.25	52.21	0.04
11-Butyldocosane	48.57	48.55	0.02
11-Decylheneicosane	57.78	57.73	0.05
12-Tricosanone	42.74	43.17	-0.43
1a,2a,4b-1,2,4-Trimethylcyclopentane	14.79	14.64	0.15
1a,2b,4a-1,2,4-Trimethylcyclopentane	14.85	14.64	0.21
1-Acetoxy-2-ethyl-3-(2-furyl)propane	20.93	21.10	-0.17
1-Acetoxy-2-ethyl-4-oxoheptane	21.60	21.82	-0.22
1-Acetoxy-2-methyl-3-(2-furyl)propane	19.11	19.27	-0.16
1-Acetoxy-2-methyl-4-oxoheptane	19.82	19.99	-0.17
1-Acetoxy-3-(2-furyl)propane	17.36	17.45	-0.09
1-Acetoxy-3-oxa-5-oxooctane	18.75	18.84	-0.09
1-Acetoxy-4-ethyl-3-oxa-5-oxooctane	22.35	22.51	-0.16
1-Acetoxy-4-oxoheptane	18.02	18.17	-0.15
1-Acetyl-3-methylpiperidine	16.22	16.16	0.06
1-Acetyl-4-piperidinone	14.42	14.44	-0.02
1-Acetylnaphthalene	21.45	21.48	-0.03
1-Acetylpiperidine	14.14	14.34	-0.20
1-Allylcyclohexanol	16.77	16.93	-0.16
1-Amino-3-methoxypropane	10.65	10.21	0.44
1-Benzosuberone	19.29	19.09	0.20

1-Benzyl-3-methylimidazolium bis(trifluoromethylsulfonyl) amide	34.03	33.98	0.05
1-Benzylpiperidine	22.04	22.26	-0.22
1-Benzylpyrrole	19.95	19.96	-0.01
1-Bromo-1,1,5-trichloropentane	18.87	18.88	-0.01
1-Bromo-1-chloroethane	9.45	9.47	-0.02
1-Bromo-1-chloropropane	11.31	11.30	0.01
1-Bromo-1-pentyne	12.41	12.35	0.06
1-Bromo-2-(trifluoromethyl)benzene	15.38	15.54	-0.16
1-Bromo-2,2-dimethylpropane	13.08	13.09	-0.01
1-Bromo-2,4-dimethylbenzene	17.42	17.33	0.09
1-Bromo-2,5-dimethylbenzene	17.24	17.33	-0.09
1-Bromo-2-butene	11.42	11.18	0.24
1-Bromo-2-butoxyethylene	15.43	15.29	0.14
1-Bromo-2-chloro-1,1,2-trifluoroethane	9.62	9.52	0.10
1-Bromo-2-chloroethane	9.46	9.49	-0.03
1-Bromo-2-chloropropane	11.47	11.31	0.16
1-Bromo-2-ethoxyethane	11.65	11.93	-0.28
1-Bromo-2-ethoxyethylene	11.78	11.61	0.17
1-Bromo-2-ethylbenzene	17.18	17.26	-0.08
1-Bromo-2-fluorobenzene	13.46	13.48	-0.02
1-Bromo-2-fluoroethane	7.53	7.56	-0.03
1-Bromo-2-isopropylacetylene	12.29	12.33	-0.04
1-Bromo-2-methoxyethane	10.08	10.08	0.00
1-Bromo-2-methylbutane	13.06	13.08	-0.02
1-Bromo-2-methylpentane	15.11	14.91	0.20
1-Bromo-2-propanol	10.04	9.99	0.05
1-Bromo-2-t-butylacetylene	14.15	14.18	-0.03
1-Bromo-2-vinylbenzene	17.36	17.14	0.22
1-Bromo-3-(trifluoromethyl)benzene	15.48	15.54	-0.06
1-Bromo-3,3-dichlorobutane	15.06	15.08	-0.02
1-Bromo-3,4-dimethylbenzene	17.12	17.33	-0.21
1-Bromo-3,5-dimethylbenzene	17.06	17.33	-0.27
1-Bromo-3-chloropropane	11.23	11.33	-0.10
1-Bromo-3-ethylbenzene	17.23	17.26	-0.03
1-Bromo-3-fluorobenzene	13.58	13.48	0.10
1-Bromo-3-fluoropropane	9.36	9.39	-0.03
1-Bromo-3-methyl-2-butene	13.28	13.04	0.24
1-Bromo-3-methylcyclohexane	16.23	15.92	0.31
1-Bromo-3-vinylbenzene	17.50	17.14	0.36
1-Bromo-4-(hexyloxy)benzene	25.44	25.29	0.15
1-Bromo-4-(trifluoromethyl)benzene	15.50	15.54	-0.04

1-Bromo-4-chlorobenzene	15.41	15.43	-0.02
1-Bromo-4-chlorobutane	13.16	13.16	0.00
1-Bromo-4-ethoxybenzene	18.09	17.95	0.14
1-Bromo-4-ethylbenzene	17.21	17.26	-0.05
1-Bromo-4-fluorobenzene	13.47	13.48	-0.01
1-Bromo-4-isopropylbenzene	19.32	19.08	0.24
1-Bromo-4-methylpentane	15.02	14.91	0.11
1-Bromo-4-vinylbenzene	17.62	17.14	0.48
1-Bromo-5,5-dichlorohexane	18.94	18.75	0.19
1-Bromo-6-fluorohexane	14.89	14.90	-0.01
1-Bromo-7,7-dichlorooctane	22.44	22.42	0.02
1-bromo-9-chloro-5-nonanone	22.27	22.44	-0.17
1-Bromobutane	11.22	11.26	-0.04
1-Bromodecane	22.26	22.27	-0.01
1-Bromododecane	25.94	25.94	0.00
1-Bromoheptadecane	35.13	35.12	0.01
1-Bromohexadecane	33.29	33.28	0.01
1-Bromonaphthalene	20.45	20.64	-0.19
1-Bromononane	20.43	20.43	0.00
1-Bromooctadecane	36.97	36.95	0.02
1-Bromooctane	18.59	18.60	-0.01
1-Bromopentadecane	31.53	31.45	0.08
1-Bromopentane	13.07	13.09	-0.02
1-Bromopropane	9.39	9.42	-0.03
1-Bromotetradecane	29.62	29.61	0.01
1-Bromotridecane	27.79	27.78	0.01
1-Bromoundecane	24.12	24.11	0.01
1-Butanethiol	11.28	11.23	0.05
1-Butanol	8.78	8.75	0.03
1-Butene	7.97	8.07	-0.10
1-Butoxy-2-propanol	14.94	14.93	0.01
1-Butoxy-4-methylbenzene	20.70	20.52	0.18
1-Butoxycyclohexene	18.80	18.83	-0.03
1-Butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide	32.30	32.31	-0.01
1-Butyl-1-methylpyrrolidinium 2-acryloamido-2- methylpropanesulfonate	36.26	35.98	0.28
1-Butyl-1-methylpyrrolidinium acetate	21.80	22.09	-0.29
1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide	30.48	30.47	0.01
1-Butyl-1-methylpyrrolidinium dicyanamide	23.83	23.56	0.27
1-Butyl-1-methylpyrrolidinium methylsulfate	24.15	23.97	0.18



1-Butyl-1-methylpyrrolidinium trifluoromethanesulfonate	23.96	23.81	0.15
1-Butyl-2,3-dimethylimidazolium bis(trifluoromethanesulfonyl) amide	31.45	31.47	-0.02
1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	20.76	20.68	0.08
1-Butyl-2-methylpyridinium tetrafluoroborate	21.19	21.24	-0.05
1-Butyl-2-pyridone	18.12	17.68	0.44
1-Butyl-3-(2-cyanoethyl)-imidazolium chloride	22.96	23.09	-0.13
1-Butyl-3-(2-cyanoethyl)imidazolium thiocyanate	26.58	26.60	-0.02
1-Butyl-3-ethylimidazolium bis(trifluoromethylsulfonyl) amide	31.49	31.57	-0.08
1-Butyl-3-ethylimidazolium triflate	24.98	24.91	0.07
1-Butyl-3-methylimidazolium 2-acryloamido-2- methylpropanesulfonate	35.09	35.26	-0.17
1-Butyl-3-methylimidazolium acetate	21.48	21.37	0.11
1-Butyl-3-methylimidazolium bis(perfluorobutanesulfonyl) amide	41.78	41.80	-0.02
1-Butyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	29.73	29.75	-0.02
1-Butyl-3-methylimidazolium dicyanoamide	22.91	22.84	0.07
1-Butyl-3-methylimidazolium glycine	23.15	22.73	0.42
1-Butyl-3-methylimidazolium hexafluorophosphate	20.40	20.44	-0.04
1-Butyl-3-methylimidazolium methosulfate	23.22	23.25	-0.03
1-Butyl-3-methylimidazolium octylsulfate	36.27	36.11	0.16
1-Butyl-3-methylimidazolium perfluorobutylsulfonate	29.07	29.11	-0.04
1-Butyl-3-methylimidazolium tetracyanoborate	26.89	26.90	-0.01
1-Butyl-3-methylimidazolium tetrafluoroborate	18.95	18.96	-0.01
1-Butyl-3-methylimidazolium thiocyanate	22.91	23.03	-0.12
1-Butyl-3-methylimidazolium threoninate	27.15	26.94	0.21
1-Butyl-3-methylimidazolium tricyanomethanide	25.90	25.92	-0.02
1-Butyl-3-methylimidazolium trifluoromethylsulfonate	22.96	23.09	-0.13
1-Butyl-4-methylpyridinium tetrafluoroborate	21.41	21.34	0.07
1-Butylamine	9.55	9.55	0.00
1-Butylnaphthalene	25.03	25.04	-0.01
1-Butylphosphine	12.17	12.15	0.02
1-Butylpyridinium 2-acryloamido-2- methylpropanesulfonate	36.08	35.74	0.34
1-Butylpyridinium bis(fluorosulfonyl) amide	25.61	25.63	-0.02
1-Butylpyridinium dicyanamide	23.34	23.31	0.03
1-Butylpyridinium tetrafluoroborate	19.42	19.44	-0.02
1-Butyltetrahydrothiophenium dicyanamide	23.62	23.71	-0.09
1-Chloro-1,2-epoxycyclohexane	12.97	12.91	0.06

1-Chloro-1,2-epoxycyclopentane	11.02	11.07	-0.05
1-Chloro-1,3-butadiene	10.22	9.85	0.37
1-Chloro-1-ethoxyethane	10.93	10.81	0.12
1-Chloro-1-phenyl-2-propene	17.83	17.85	-0.02
1-Chloro-2-(methylthio)ethane	11.29	11.31	-0.02
1-Chloro-2-(trichloromethyl)benzene	20.07	20.16	-0.09
1-Chloro-2,2-difluoropropane	8.18	8.41	-0.23
1-Chloro-2,2-dimethylpropane	11.94	11.92	0.02
1-Chloro-2,3-epoxycyclohexane	12.85	12.73	0.12
1-Chloro-2,3-epoxycyclopentane	11.04	10.89	0.15
1-Chloro-2,4-bis(trifluoromethyl)benzene	16.20	16.46	-0.26
1-Chloro-2,4-dinitrobenzene	17.98	17.71	0.27
1-Chloro-2-butanol	10.62	10.66	-0.04
1-Chloro-2-butyne	9.43	9.50	-0.07
1-Chloro-2-fluorobenzene	12.27	12.38	-0.11
1-Chloro-2-fluoroethane	6.41	6.39	0.02
1-Chloro-2-isopropylbenzene	17.93	17.98	-0.05
1-Chloro-2-methoxyethane	9.00	8.92	0.08
1-Chloro-2-methyl-1-propene	9.93	10.00	-0.07
1-Chloro-2-nitro-4-(trifluoromethyl)benzene	17.09	17.08	0.01
1-Chloro-2-phenylethane	16.05	16.16	-0.11
1-Chloro-2-propanol	8.86	8.82	0.04
1-Chloro-3-(1-methylethoxy)-2-propanol	14.53	15.00	-0.47
1-Chloro-3-(trifluoromethyl)benzene	14.28	14.44	-0.16
1-Chloro-3-ethylbenzene	16.08	16.17	-0.09
1-Chloro-3-fluoro-2-methylbenzene	14.21	14.29	-0.08
1-Chloro-3-fluorobenzene	12.28	12.38	-0.10
1-Chloro-3-iodopropane	13.50	13.36	0.14
1-Chloro-3-methyl-2-butene	11.98	11.88	0.10
1-Chloro-4-((chloromethyl)thio)benzene	19.60	19.53	0.07
1-Chloro-4-(trifluoromethyl)benzene	14.23	14.44	-0.21
1-Chloro-4-ethoxybenzene	16.91	16.85	0.06
1-Chloro-4-fluorobutane	10.05	10.06	-0.01
1-Chloro-4-iodobutane	15.22	15.20	0.02
1-Chloro-4-isopropylbenzene	18.01	17.98	0.03
1-Chloro-4-nitro-2-(trifluoromethyl)benzene	17.46	17.08	0.38
1-Chloro-4-tert-butylbenzene	19.92	19.83	0.09
1-Chloro-5-fluoropentane	11.90	11.90	0.00
1-Chlorobut-1-yn-3-ene	9.47	9.62	-0.15
1-Chlorobutane	10.10	10.09	0.01
1-Chlorocyclohexene	12.66	12.88	-0.22
1-Chlorodecane	21.15	21.10	0.05

1-Chlorododecane	24.83	24.77	0.06
1-Chloroheptane	15.62	15.60	0.02
1-Chlorohexadecane	32.20	32.12	0.08
1-Chlorohexane	13.78	13.76	0.02
1-Chloronaphthalene	19.37	19.54	-0.17
1-Chlorononane	19.13	19.27	-0.14
1-Chlorooctadecane	35.89	35.79	0.10
1-Chlorooctane	17.46	17.43	0.03
1-Chloropentane	11.94	11.93	0.01
1-Chloropropane	8.25	8.26	-0.01
1-Chlorotetradecane	28.52	28.45	0.07
1-Crotyl-2-pyridone	17.98	17.60	0.38
1-Cyanonaphthalene	19.49	19.46	0.03
1-Cyclohexene-1-carboxaldehyde	13.26	13.00	0.26
1-Cyclohexene-1-carboxylic acid	13.04	13.43	-0.39
1-Cyclohexyl-4-hexyldecane	40.37	40.35	0.02
1-Cyclopentene-1-carboxaldehyde	11.30	11.17	0.13
1-Cyclopropyl-1,4-cyclohexadiene	15.37	15.52	-0.15
1-Cyclopropylcyclohexene	15.74	15.60	0.14
1-Decanethiol	22.12	22.24	-0.12
1-Decen-3-yne	18.78	18.48	0.30
1-Decene	19.05	19.08	-0.03
1-Decyl hydroperoxide	20.81	20.68	0.13
1-Decyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	40.79	40.76	0.03
1-Decyl-3-methylimidazolium tetracyanoborate	37.92	37.92	0.00
1-Decyl-3-methylimidazolium tricyanomethanide	36.96	36.93	0.03
1-Decylnaphthalene	36.01	36.06	-0.05
1-Decylphosphine	23.14	23.16	-0.02
1-Decyne	18.36	18.39	-0.03
1-Dimethylamino-2-propyne	10.69	10.76	-0.07
1-Docosanoic acid	42.16	41.86	0.30
1-Dodecanol	23.51	23.43	0.08
1-Dodecen-3-yne	22.48	22.15	0.33
1-Dodecene	22.73	22.75	-0.02
1-Dodecyl-2-methylcyclohexane	34.93	34.84	0.09
1-Dodecyl-3-methylcyclohexane	35.02	34.84	0.18
1-Dodecyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	44.43	44.43	0.00
1-Dodecylphosphine	26.65	26.83	-0.18
1-Dodecylpiperidine	32.77	32.71	0.06
1-Dodecyne	22.04	22.06	-0.02

1-Eicosene	37.48	37.43	0.05
1-Ethoxy-1,1,2,2-tetrafluoroethane	8.88	9.16	-0.28
1-Ethoxy-2-nitrobenzene	17.53	17.59	-0.06
1-Ethoxycyclohexene	14.94	15.16	-0.22
1-Ethoxynaphthalene	21.89	22.06	-0.17
1-Ethyl-1H-pyrrole	11.98	12.06	-0.08
1-Ethyl-1-methylcyclopentane	14.71	14.67	0.04
1-Ethyl-1-methylcyclopropane	11.32	11.00	0.32
1-Ethyl-1-phenylhydrazine	17.43	17.25	0.18
1-Ethyl-2,3-dimethylimidazolium bis(trifluoromethanesulfonyl) amide	27.72	27.80	-0.08
1-Ethyl-2,4,5-trimethylbenzene	19.82	19.97	-0.15
1-Ethyl-2-isopropylbenzene	19.73	19.82	-0.09
1-Ethyl-2-propyn-1-ylether	9.80	9.89	-0.09
1-Ethyl-2-pyrrolidinemethanamine	15.88	15.69	0.19
1-Ethyl-3-methylimidazolium 1,1,2,2- tetrafluoroethanesulfonate	21.37	21.31	0.06
1-Ethyl-3-methylimidazolium acetate	17.82	17.70	0.12
1-Ethyl-3-methylimidazolium aminoacetate	18.90	19.06	-0.16
1-Ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	26.07	26.08	-0.01
1-Ethyl-3-methylimidazolium dicyanamide	19.17	19.17	0.00
1-Ethyl-3-methylimidazolium diethylphosphate	25.59	25.51	0.08
1-Ethyl-3-methylimidazolium dimethylphosphate	21.87	21.81	0.06
1-Ethyl-3-methylimidazolium ethosulfate	21.47	21.43	0.04
1-Ethyl-3-methylimidazolium imidodisulfurylfluoride	21.43	21.48	-0.05
1-Ethyl-3-methylimidazolium L-alanine	20.65	20.87	-0.22
1-Ethyl-3-methylimidazolium L-proline	23.32	23.67	-0.35
1-Ethyl-3-methylimidazolium L-serine	21.43	21.43	0.00
1-Ethyl-3-methylimidazolium methanesulfonate	19.21	19.30	-0.09
1-Ethyl-3-methylimidazolium methylsulfate	19.27	19.58	-0.31
1-Ethyl-3-methylimidazolium taurinate	22.36	22.58	-0.22
1-Ethyl-3-methylimidazolium tetracyanoborate	23.30	23.23	0.07
1-Ethyl-3-methylimidazolium tetrafluoroborate	15.34	15.29	0.05
1-Ethyl-3-methylimidazolium thiocyanate	19.15	19.36	-0.21
1-Ethyl-3-methylimidazolium threoninate	23.33	23.26	0.07
1-Ethyl-3-methylimidazolium tricyanomethide	22.15	22.25	-0.10
1-Ethyl-3-methylimidazolium trifluoromethylsulfonate	19.39	19.42	-0.03
1-Ethyl-3-methylpyridinium bis(fluorosulfonyl) amide	23.85	23.86	-0.01
1-Ethyl-3-methylpyridinium ethylsulfate	23.86	23.81	0.05

1-Ethyl-3-propylimidazolium bis(trifluoromethanesulfonyl) amide	29.71	29.73	-0.02
1-Ethyl-4-methoxybenzene	16.83	16.84	-0.01
1-Ethyladamantane	20.24	20.27	-0.03
1-Ethylcyclohexene	14.54	14.63	-0.09
1-Ethylcyclopentene	12.69	12.80	-0.11
1-Ethylmorpholinium tetrafluoroborate	16.18	15.81	0.37
1-Ethyl-naphthalene	21.19	21.37	-0.18
1-Ethylpiperidine	14.58	14.36	0.22
1-Ethylpyridinium bis(fluorosulfonyl) amide	21.87	21.96	-0.09
1-Ethylpyridinium ethylsulfate	21.92	21.90	0.02
1-Ethylpyridinium triflate	19.84	19.89	-0.05
1-Ethyltetrahydrothiophenium dicyanamide	20.16	20.04	0.12
1-Ethynylcyclohexanamine	15.24	15.21	0.03
1-Ethynylcyclohexanol	14.22	14.41	-0.19
1-Ethynylcyclopentanol	12.78	12.58	0.20
1-Fluoro-2-(trichloromethyl)benzene	18.36	18.21	0.15
1-Fluoro-4-(trifluoromethyl)benzene	12.26	12.49	-0.23
1-Fluorobutane	8.11	8.16	-0.05
1-Fluorodecane	19.15	19.17	-0.02
1-Fluorododecane	22.83	22.84	-0.01
1-Fluoroheptane	13.63	13.66	-0.03
1-Fluorohexane	11.79	11.83	-0.04
1-Fluoronaphthalene	17.33	17.59	-0.26
1-Fluorononane	17.34	17.33	0.01
1-Fluorooctane	15.47	15.50	-0.03
1-Fluoropentane	9.95	9.99	-0.04
1-Fluoropropane	6.27	6.32	-0.05
1-Fluorotetradecane	26.57	26.51	0.06
1-Fluoroundecane	21.00	21.01	-0.01
1-Formyl-naphthalene	19.65	19.74	-0.09
1-Formylpiperidine	12.55	12.56	-0.01
1-Heptadecene	31.93	31.93	0.00
1-Heptadecylamine	33.42	33.41	0.01
1-Heptanethiol	16.79	16.74	0.05
1-Heptanol	14.33	14.25	0.08
1-Hepten-3-yne	13.28	12.98	0.30
1-Hepten-4-ol	14.08	14.14	-0.06
1-Heptene	13.53	13.57	-0.04
1-Heptyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	34.94	35.26	-0.32
1-Heptyl-3-methylimidazolium hexafluorophosphate	25.94	25.94	0.00

1-Heptylhydroperoxide	15.21	15.18	0.03
1-Heptylnaphthalene	30.50	30.55	-0.05
1-Heptyltrifluorosilane	16.38	16.28	0.10
1-Heptyne	12.86	12.89	-0.03
1-Hexadecylphosphine	34.19	34.17	0.02
1-Hexadecyne	29.40	29.40	0.00
1-Hexanethiol	14.94	14.90	0.04
1-Hexanol	12.54	12.42	0.12
1-Hexen-3-ol	12.29	12.30	-0.01
1-Hexen-3-yne	11.44	11.14	0.30
1-Hexen-5-one	11.77	11.84	-0.07
1-Hexene	11.70	11.74	-0.04
1-Hexyl-1,2,3,4-tetrahydronaphthalene	28.08	28.14	-0.06
1-Hexyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl) amide	34.59	34.14	0.45
1-Hexyl-3,5-dimethylpyridinium bis(trifluoromethylsulfonyl)amide	37.88	37.71	0.17
1-Hexyl-3-methylimidazolium acetate	25.19	25.04	0.15
1-Hexyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	33.39	33.42	-0.03
1-Hexyl-3-methylimidazolium chloride	23.31	23.19	0.12
1-Hexyl-3-methylimidazolium dicyanoamide	26.63	26.51	0.12
1-Hexyl-3-methylimidazolium hexafluorophosphate	24.06	24.11	-0.05
1-Hexyl-3-methylimidazolium tetracyanoborate	30.48	30.57	-0.09
1-Hexyl-3-methylimidazolium tetrafluoroborate	22.56	22.63	-0.07
1-Hexyl-3-methylimidazolium thiocyanate	27.02	26.70	0.32
1-Hexyl-3-methylimidazolium tricyanomethanide	29.60	29.59	0.01
1-Hexylhydroperoxide	13.33	13.34	-0.01
1-Hexyl-naphthalene	28.65	28.72	-0.07
1-Hexylphosphine	15.86	15.82	0.04
1-Hexylpyridinium bis(fluorosulfonyl) amide	29.31	29.30	0.01
1-Hexyn-3-ol	11.64	11.61	0.03
1-Hexyne	11.00	11.05	-0.05
1H-Pentadecafluoroheptane	14.38	14.52	-0.14
1H-Pyrazole	7.23	7.36	-0.13
1-Hydroxy-2-butanone	8.59	8.86	-0.27
1-Hydroxycyclohexanecarbonitrile	13.59	13.30	0.29
1-Hydroxytetralin	17.37	17.71	-0.34
1-Indanamine	16.48	16.64	-0.16
1-Indanone	15.50	15.42	0.08
1-Iodo-2,2-dimethylpropane	15.17	15.12	0.05
1-Iodo-2,4-dimethylbenzene	19.35	19.31	0.04

1-Iodo-2,5-dimethylbenzene	19.44	19.31	0.13
1-Iodo-2,6-dimethylbenzene	19.57	19.31	0.26
1-Iodo-2-triazobenzene	19.05	18.97	0.08
1-Iodobutane	13.28	13.30	-0.02
1-Iododecane	24.24	24.31	-0.07
1-Iodododecane	27.98	27.98	0.00
1-Iodoheptafluoropropane	11.51	11.69	-0.18
1-Iodoheptane	18.80	18.80	0.00
1-Iodohexadecane	35.48	35.32	0.16
1-Iodohexane	16.96	16.97	-0.01
1-Iodonaphthalene	22.44	22.61	-0.17
1-Iodononane	22.49	22.47	0.02
1-Iodooctadecane	39.03	38.99	0.04
1-Iodooctane	20.64	20.64	0.00
1-Iodopentane	15.12	15.13	-0.01
1-Isoamyloxycyclohexene	20.64	20.65	-0.01
1-Isobutyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide	30.53	30.46	0.07
1-Isobutyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	29.70	29.73	-0.03
1-Isobutyl-3-methylpyridinium bis(trifluoromethylsulfonyl)amide	32.20	32.12	0.08
1-Isopropoxy-2-propanol	13.12	13.10	0.02
1-Isopropyl-4-nitrobenzene	18.86	18.72	0.14
1-Isopropylnaphthalene	23.04	23.19	-0.15
1-Methoxy-2-crotyl-4-methylbenzene	22.36	22.34	0.02
1-Methoxy-2-methyl-4,6-dicrotylbenzene	29.40	29.67	-0.27
1-Methoxy-2-methyl-4-crotylbenzene	22.31	22.34	-0.03
1-Methoxy-2-propanol	9.07	9.41	-0.34
1-Methoxy-2-propanone	8.79	8.95	-0.16
1-Methoxy-4-methyl-2,6-di(3-hexen-2-yl)benzene	36.95	36.98	-0.03
1-Methoxy-4-Methyl-2,6-dicrotylbenzene	29.50	29.67	-0.17
1-Methoxy-4-propylbenzene	18.66	18.67	-0.01
1-Methoxy-5-heptanol	16.72	16.75	-0.03
1-Methoxy-5-undecanol	24.09	24.09	0.00
1-Methoxybut-1-yn-3-ene	10.24	10.01	0.23
1-Methoxycyclohexene	13.24	13.32	-0.08
1-Methoxynaphthalene	20.18	20.22	-0.04
1-Methyl-1-(2',3'-epoxypropyl)-2-oxopyrrolidinium chloride	19.57	19.74	-0.17
1-Methyl-1,3-cyclopentadiene	10.56	10.88	-0.32
1-Methyl-1-butylhydrazine	12.95	12.92	0.03

1-Methyl-1-decylpyrrolidinium bis(trifluoromethanesulfonyl) amide	41.58	41.48	0.10
1-Methyl-1H-indene	17.24	17.05	0.19
1-Methyl-1H-pyrazole	9.29	9.42	-0.13
1-Methyl-1-isobutylhydrazine	12.95	12.90	0.05
1-Methyl-1-isopropylhydrazine	11.00	11.06	-0.06
1-Methyl-1-phenylhydrazine	15.25	15.43	-0.18
1-Methyl-1-propylhydrazine	11.09	11.08	0.01
1-Methyl-1-propylpiperidinium bis(trifluoromethylsulfonyl)amide	30.48	30.47	0.01
1-Methyl-1-propylpyrrolidinium bis(fluorosulfonyl) amide	24.20	24.04	0.16
1-Methyl-1-propylpyrrolidinium bis(trifluoromethanesulfonyl) amide	28.74	28.64	0.10
1-Methyl-2-ethyl-5-propylpyrrole	19.36	19.40	-0.04
1-Methyl-2-ethyl-5-propylpyrrolidine	19.64	19.83	-0.19
1-Methyl-2-piperidone	12.46	12.52	-0.06
1-Methyl-2-propyl-4-ethylpyrrole	19.51	19.44	0.07
1-Methyl-2-propyl-4-ethyl-pyrrolidine	19.80	19.84	-0.04
1-Methyl-2-pyrrolidonium tetrafluoroborate	14.68	14.94	-0.26
1-Methyl-3-hexylimidazolium threoninate	30.81	30.61	0.20
1-Methyl-3-pentylimidazolium threoninate	28.96	28.77	0.19
1-Methyl-3-phenoxybenzene	22.89	22.93	-0.04
1-Methyl-3-phenylpropylamine	19.21	19.26	-0.05
1-Methyl-3-piperidinol	13.28	13.10	0.18
1-Methyl-3-propylimidazolium threoninate	25.27	25.10	0.17
1-Methyl-4-(1-methylvinyl)benzene	18.07	17.90	0.17
1-Methyl-4-(1-pentenyl-2-oxy)benzene	22.15	22.24	-0.09
1-Methyl-4-(phenylthio)benzene	25.47	25.46	0.01
1-Methyl-4-benzylbenzene	23.80	24.06	-0.26
1-Methyl-4-cyclopropyl-1,4-cyclohexadiene	17.24	17.39	-0.15
1-Methyl-4-isopropyl-2-nitrobenzene	20.43	20.62	-0.19
1-Methyl-4-isopropyl-7-oxabicyclo[2.2.1]heptane	18.48	18.12	0.36
1-Methyl-4-isopropylcyclohexanol	18.92	18.86	0.06
1-Methyl-4-isopropylcyclohexene	18.19	18.27	-0.08
1-Methyl-4-piperidone	12.61	12.65	-0.04
1-Methyl-4-vinylcyclohexene	15.90	16.33	-0.43
1-Methylanthracene	26.45	26.66	-0.21
1-Methylbenzimidazole	16.12	16.27	-0.15
1-Methylcyclohexanol	13.47	13.39	0.08
1-Methylcyclohexene	12.65	12.80	-0.15
1-Methylcyclopentanol	11.64	11.55	0.09



1-Methylcyclopentene	10.90	10.96	-0.06
1-Methylimidazole	9.22	9.23	-0.01
1-Methylmorpholinium tetrafluoroborate	14.23	14.10	0.13
1-Methylnaphthalene	19.30	19.54	-0.24
1-Methylpiperidinium tetrafluoroborate	15.00	15.27	-0.27
1-Methylpyridinium methylsulfate	18.25	18.34	-0.09
1-Methylpyrrole	10.12	10.24	-0.12
1-Methylpyrrolidinium tetrafluoroborate	13.70	13.43	0.27
1-Methyltetralin	18.84	18.97	-0.13
1-Naphthalenethiol	20.68	20.80	-0.12
1-Naphthol	18.33	18.33	0.00
1-Naphthylamine	19.34	19.25	0.09
1-Nitrobutane	10.41	10.46	-0.05
1-Nitrohexane	14.21	14.14	0.07
1-Nitrooctane	17.52	17.81	-0.29
1-Nitropentane	12.27	12.30	-0.03
1-Nitropropane	8.59	8.63	-0.04
1-Nitropropylene	8.74	8.33	0.41
1-Nonadecene	35.62	35.60	0.02
1-Nonanol	17.96	17.93	0.03
1-Nonen-3-ol	17.97	17.81	0.16
1-Nonen-3-yne	16.97	16.65	0.32
1-Nonene	17.67	17.24	0.43
1-Nonyl hydroperoxide	18.81	18.85	-0.04
1-Nonyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	38.87	38.93	-0.06
1-Nonyl-3-methylimidazolium hexafluorophosphate	29.63	29.62	0.01
1-Nonylnaphthalene	34.17	34.22	-0.05
1-Nonylphosphine	21.30	21.33	-0.03
1-Nonyne	16.33	16.56	-0.23
1-Octadecene	33.75	33.76	-0.01
1-Octadecylphosphine	37.88	37.84	0.04
1-Octanethiol	18.62	18.57	0.05
1-Octanol	16.13	16.09	0.04
1-Octen-3-ol	15.93	15.97	-0.04
1-Octen-3-yne	15.13	14.81	0.32
1-Octyl hydroperoxide	17.03	17.01	0.02
1-Octyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	37.11	37.09	0.02
1-Octyl-3-methylimidazolium chloride	26.88	26.86	0.02
1-Octyl-3-methylimidazolium hexafluorophosphate	27.87	27.78	0.09
1-Octyl-3-methylimidazolium tetracyanoborate	34.25	34.24	0.01

1-Octyl-3-methylimidazolium tetrafluoroborate	26.26	26.30	-0.04
1-Octyl-3-methylimidazolium tricyanomethanide	33.33	33.26	0.07
1-Octyl-3-methylpyridinium tetrafluoroborate	28.83	28.68	0.15
1-Octylnaphthalene	32.35	32.39	-0.04
1-Octylphosphine	19.45	19.49	-0.04
1-Octylpyridinium bis(trifluoromethylsulfonyl)amide	37.73	37.57	0.16
1-Octyne	14.69	14.72	-0.03
1-Pentadecanoic acid	29.19	29.01	0.18
1-Pentadecene	28.25	28.26	-0.01
1-Pentadecyne	27.56	27.57	-0.01
1-Pentanethiol	12.98	13.07	-0.09
1-Pentanol	10.63	10.58	0.05
1-Penten-3-ol	10.38	10.46	-0.08
1-Penten-3-one	9.95	10.01	-0.06
1-Penten-3-yne	9.51	9.31	0.20
1-Penten-4-yne	8.84	9.09	-0.25
1-Pentene	9.85	9.90	-0.05
1-Pentyl-3-methylimidazolium acetate	23.39	23.21	0.18
1-Pentyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	31.54	31.59	-0.05
1-Pentyl-3-methylimidazolium hexafluorophosphate	22.24	22.27	-0.03
1-Pentyl-3-methylimidazolium tetrafluoroborate	20.71	20.80	-0.09
1-Pentylnaphthalene	26.80	26.88	-0.08
1-Pentylphosphine	14.04	13.98	0.06
1-Pentylpyridinium dicyanamide	25.15	25.15	0.00
1-Pentyne	9.17	9.22	-0.05
1-Phenoxy-2-propanol	17.35	17.34	0.01
1-Phenoxy-2-propanone	16.67	16.89	-0.22
1-Phenyl-1,2-propanedione	16.66	16.30	0.36
1-Phenyl-1-butanol	18.40	18.49	-0.09
1-Phenyl-1-dodecanone	32.75	32.71	0.04
1-Phenyl-1-propanol	16.47	16.65	-0.18
1-Phenyl-1-propanone	16.26	16.20	0.06
1-Phenyl-2,3,5-trimethylpyrazolium methylsulfonate	27.26	27.49	-0.23
1-Phenyl-2-butanone	17.83	18.03	-0.20
1-Phenyl-2-buten-1-one	18.35	17.95	0.40
1-Phenyl-2-butene	17.75	17.85	-0.10
1-Phenyl-2-butyl-3,5-dimethylpyrazolium methylsulfonate	32.77	32.87	-0.10
1-Phenyl-2-heptyl-3,5-dimethylpyrazolium methylsulfonate	38.69	38.38	0.31

1-Phenyl-2-hexyl-3,5-dimethylpyrazolium methanesulfonate	36.72	36.54	0.18
1-Phenyl-2-methyl-2-propanol	18.42	18.46	-0.04
1-Phenyl-2-methylpropanol	18.32	18.47	-0.15
1-Phenyl-2-pentanone	19.67	19.87	-0.20
1-Phenyl-2-pentyl-3,5-dimethylpyrazolium methanesulfonate	34.55	34.71	-0.16
1-Phenyl-2-propanol	16.53	16.65	-0.12
1-Phenyl-3-butene	17.63	17.80	-0.17
1-Phenyl-3-hexanone	21.48	21.70	-0.22
1-Phenyl-3-pentanone	19.65	19.87	-0.22
1-Phenyl-4-hexyl-3-decene	39.77	39.90	-0.13
1-Phenyl-4-hexyldecane	39.89	39.93	-0.04
1-Phenylallyl alcohol	16.30	16.53	-0.23
1-Phenylcyclohexene	20.76	20.70	0.06
1-Phenyldodecane	32.59	32.61	-0.02
1-Phenylimidazole	17.21	16.95	0.26
1-Phenylnaphthalene	27.48	27.44	0.04
1-Phenylpiperazine	20.36	20.20	0.16
1-Phenylpropargyl alcohol	15.68	15.84	-0.16
1-Phenylpyrrolidine	19.11	18.86	0.25
1-Piperazineethanamine	15.25	15.22	0.03
1-Piperidinamine	12.05	12.05	0.00
1-Piperidineethanol	14.86	14.92	-0.06
1-Piperidinepropanenitrile	16.19	16.11	0.08
1-Propanesulfonylchloride	12.03	11.84	0.19
1-Propanethiol	9.42	9.39	0.03
1-Propanol	6.98	6.91	0.07
1-Propionaphthone	23.22	23.32	-0.10
1-Propoxy-2-propanol	13.14	13.09	0.05
1-Propoxycyclohexene	17.04	17.00	0.04
1-Propyl-3-methylimidazolium acetate	19.57	19.53	0.04
1-Propyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	27.94	27.91	0.03
1-Propyl-3-methylimidazolium tetrafluoroborate	17.08	17.12	-0.04
1-Propylamine	7.69	7.71	-0.02
1-Propylcyclopentanol	15.11	15.22	-0.11
1-Propylnaphthalene	23.09	23.21	-0.12
1-Propylpyridinium dicyanamide	21.50	21.48	0.02
1-Propylpyridinium tetrafluoroborate	17.58	17.60	-0.02
1-Propynylbenzene	15.88	15.50	0.38
1-Propyronitrile-3-butylimidazolium bromide	24.81	24.72	0.09

1-Propyronitrile-3-hexylimidazolium bromide	28.44	28.39	0.05
1-Propyronitrile-3-octylimidazolium bromide	31.91	32.06	-0.15
1-Pyrrolidineethanamine	13.98	13.89	0.09
1-Pyrrolidineethanol	13.10	13.09	0.01
1-t-Amylnaphthalene	26.91	26.87	0.04
1-t-Butyl-4-methoxybenzene	25.81	26.02	-0.21
1-t-Butylnaphthalene	24.97	25.04	-0.07
1-Tetradecanethiol	29.49	29.58	-0.09
1-Tetradecene	26.23	26.42	-0.19
1-Tetradecylamine	27.94	27.90	0.04
1-Tetradecylphosphine	30.47	30.50	-0.03
1-Tetralone	17.23	17.26	-0.03
1-Tridecene	24.58	24.58	0.00
1-Tridecyne	23.59	23.90	-0.31
1-Undecanol	21.66	21.60	0.06
1-Undecene	20.89	20.91	-0.02
1-Undecyne	20.20	20.23	-0.03
1-Vinyl-3-nitrobenzene	17.12	16.78	0.34
1-Vinyl-4-fluorobenzene	14.29	14.09	0.20
1-Vinylcyclohexene	14.42	14.51	-0.09
2-((2-Methylphenyl)amino)ethanol	18.16	18.36	-0.20
2-(1,1,2,2-Tetrafluoroethoxy)ethanol	9.56	9.72	-0.16
2-(1-Ethylpropyl)pyridine	18.88	18.90	-0.02
2-(1-Hydroxybutyl)furan	15.69	15.48	0.21
2-(1-Hydroxyethyl)-thiophene	14.27	14.21	0.06
2-(1-Hydroxyisobutyl)furan	15.31	15.47	-0.16
2-(1-Iodoethyl)-1,3-dioxolane-4-methanol	18.05	18.09	-0.04
2-(1-Methyl-3-butenyl)-4-cresol	22.10	22.23	-0.13
2-(1-Methylvinyl)aniline	17.79	17.61	0.18
2-(1-Vinyloxyethyl)-thiophene	17.62	17.72	-0.10
2-(2-(1-Methylethoxy)ethyl)pyridine	19.65	19.59	0.06
2-(2-(2-Butoxyethoxy)ethoxy)ethanol	21.74	21.77	-0.03
2-(2-(Diethylamino)ethoxy)ethanol	18.16	18.27	-0.11
2-(2-(Methylthio)ethylthio)ethanol	16.74	16.78	-0.04
2-(2-Butoxyethoxy)ethyl acetate	21.07	21.24	-0.17
2-(2-Chloroethoxy)ethanol	11.31	11.32	-0.01
2-(2-Hydroxyethyl)-thiophene	14.13	14.21	-0.08
2-(2-Methoxyethoxy)ethanol	11.80	11.91	-0.11
2-(2-Methoxyethyl)pyridine	16.12	15.90	0.22
2-(2-Methylpropoxy)ethanol	13.16	13.07	0.09
2-(2-Pyridyl)ethanol	13.97	13.97	0.00
2-(2-Pyridyl)ethylamine	14.72	14.77	-0.05

2-(2-Vinyloxyethyl)-thiophene	17.74	17.71	0.03
2-(3-Methyl-6-hydroxyphenyl)-3-hexene	24.06	24.11	-0.05
2-(3-Methyl-6-methoxyphenyl)-3-hexene	26.04	25.99	0.05
2-(3-Pentenyl)pyridine	18.83	18.84	-0.01
2-(4-Ethylphenyl)ethanol	18.49	18.56	-0.07
2-(Acetyloxy)-1-phenylethanone	18.71	18.73	-0.02
2-(Allyloxy)ethanol	11.04	11.13	-0.09
2-(Benzylamino)ethanol	17.74	17.98	-0.24
2-(Benzyloxy)ethanol	17.33	17.32	0.01
2-(Bromomethoxy)butane	14.05	14.23	-0.18
2-(Bromomethoxy)heptane	19.86	19.74	0.12
2-(Bromomethoxy)octane	21.85	21.58	0.27
2-(Bromomethyl)tetrahydrofuran	12.77	12.92	-0.15
2-(Butylamino)ethanol	13.85	13.76	0.09
2-(Chloromethyl)-2-methyloxirane	9.93	9.89	0.04
2-(Chloromethyl)furan	11.42	11.32	0.10
2-(Chloromethylthio)benzothiazole	23.66	23.70	-0.04
2-(Diethoxymethyl)furan	18.00	18.03	-0.03
2-(Diethylamino)ethyl acrylate	19.00	19.45	-0.45
2-(Ethylamino)ethanol	10.27	10.08	0.19
2-(Isopropylamino)ethanol	12.00	11.89	0.11
2-(Methacryloyloxy)ethyl acetoacetate	20.57	20.91	-0.34
2-(Methoxymethyl)furan	11.91	11.91	0.00
2-(Methylthio)aniline	17.54	17.24	0.30
2-(Methylthio)ethanol	9.87	9.97	-0.10
2-(Methylthiomethylthio)ethanol	14.83	14.86	-0.03
2-(Phenoxymethyl)oxirane	16.57	16.61	-0.04
2-(Phenylmethoxy)phenol	23.23	23.55	-0.32
2-(Propylamino)ethanol	12.03	11.92	0.11
2,2,2-Trifluoroethanol	5.20	5.19	0.01
2,2,3,3,4,4,4-Heptafluoro-1-butanol	9.10	9.16	-0.06
2,2,3,3,4,4,5,5-Octafluoro-1-pentanol	10.89	10.99	-0.10
2,2,3,3,4-Pentamethylpentane	18.99	19.17	-0.18
2,2,3,3-Tetrafluoro-1-propanol	6.98	7.02	-0.04
2,2,3,3-Tetramethylbutane	15.31	15.52	-0.21
2,2,3,3-Tetramethylbutanoic acid	16.10	16.15	-0.05
2,2,3,3-Tetramethylhexane	19.08	19.19	-0.11
2,2,3,3-Tetramethylpentane	17.22	17.35	-0.13
2,2,3,4,4-Pentamethylpentane	19.11	19.17	-0.06
2,2,3,4-Tetramethylhexane	19.01	19.16	-0.15
2,2,3,4-Tetramethylpentane	17.22	17.33	-0.11
2,2,3-Tribromobutane	17.40	17.47	-0.07

2,2,3-Trichloro-1,1,1,3,4,4,4-heptafluorobutane	14.13	14.20	-0.07
2,2,3-Trichlorobutyraldehyde	14.04	14.10	-0.06
2,2,3-Trimethylbutanoic acid	14.25	14.31	-0.06
2,2,3-Trimethylhexane	17.38	17.34	0.04
2,2,3-Trimethylpentane	15.43	15.51	-0.08
2,2,4,4,6,6-Hexamethylcyclotrisilazane	25.33	25.28	0.05
2,2,4,4-Tetramethylpentane	17.39	17.35	0.04
2,2,4,6,6-Pentamethylheptane	22.91	22.84	0.07
2,2,4-Trimethyl-1,3-pentanediol	16.68	16.63	0.05
2,2,4-Trimethyl-3-pentanol	16.03	16.07	-0.04
2,2,4-Trimethyl-3-pentanone	15.48	15.61	-0.13
2,2,4-Trimethylcyclopentanone	14.73	14.77	-0.04
2,2,4-Trimethylhexane	17.46	17.34	0.12
2,2,4-Trimethylpiperidine	16.16	15.97	0.19
2,2,5,5-Tetramethylhexane	19.36	19.19	0.17
2,2,5,5-Tetramethyltetrahydrofuran	15.40	15.31	0.09
2,2,5-Trimethylhexane	17.42	17.34	0.08
2,2,6,6-Tetramethyl-4-piperidinamine	18.97	19.13	-0.16
2,2,6-Trimethylcyclohexanone	16.42	16.60	-0.18
2,2,6-Trimethylheptane	19.32	19.18	0.14
2,2'-Bioxirane	8.00	7.84	0.16
2,2'-Diaminodiethylamine	12.16	12.24	-0.08
2,2-Bis(butylthio)-1-propanol	27.97	27.97	0.00
2,2-Bis(butylthio)butane	29.17	29.25	-0.08
2,2-Bis(isobutylthio)-1-propanol	28.12	27.94	0.18
2,2-Bis(isopropylthio)butane	25.33	25.57	-0.24
2,2-Bis(isopropylthio)propane	23.70	23.73	-0.03
2,2-Bis(methylthio)-hexane	22.06	21.74	0.32
2,2-Bis(propylthio)-1-propanol	24.45	24.30	0.15
2,2-Dichloro-4,4-dimethylhexane	19.27	19.34	-0.07
2,2-Dichloro-4,4-dimethylpentane	17.70	17.51	0.19
2,2-Dichloro-7,7-bis(ethoxycarbonyl)heptane	29.94	29.90	0.04
2,2-Dichlorobutane	11.76	12.01	-0.25
2,2'-Dichlorodiisopropyl ether	16.26	16.34	-0.08
2,2-Dichloroethanol	8.93	8.91	0.02
2,2-Dichloroethylsulfonyl fluoride	11.99	12.16	-0.17
2,2-Dichlorohexane	15.81	15.68	0.13
2,2-Dichloropropane	10.07	10.17	-0.10
2,2-Diethoxybutane	16.68	16.76	-0.08
2,2-Diethoxyethanamine	14.35	14.50	-0.15
2,2-Diethoxyhexane	20.24	20.43	-0.19
2,2-Diethoxypentane	18.48	18.60	-0.12

2,2-Diethoxypropane	15.12	14.93	0.19
2,2-Diethyl-5-propyltetrahydrofuran	20.87	20.84	0.03
2,2-Diethyl-5-propylthiophane	23.21	23.47	-0.26
2,2-Difluoropropane	6.26	6.50	-0.24
2,2-Dimethoxybutane	12.98	13.07	-0.09
2,2-Dimethoxyethanamine	10.85	10.80	0.05
2,2-Dimethoxy-N-methylethanamine	12.65	12.63	0.02
2,2-Dimethoxypropane	11.24	11.23	0.01
2,2-Dimethyl-1-butanol	12.40	12.41	-0.01
2,2-Dimethyl-3-ethylpentane	17.02	17.34	-0.32
2,2-Dimethyl-3-pentanol	14.19	14.25	-0.06
2,2-Dimethyl-4-(2-butylthioethoxymethyl)-1,3-dioxolane	26.91	27.07	-0.16
2,2'-Dimethylbiphenyl	24.11	24.13	-0.02
2,2-Dimethylbutanoic acid	12.42	12.49	-0.07
2,2-Dimethylcyclohexanone	14.66	14.78	-0.12
2,2-Dimethylheptane	17.41	17.36	0.05
2,2-Dimethylhexane	15.56	15.52	0.04
2,2-Dimethylnonanoic acid	21.61	21.66	-0.05
2,2-Dimethyloctadecane	37.61	37.55	0.06
2,2-Dimethyloctane	19.31	19.19	0.12
2,2-Dimethyloctanoic acid	19.78	19.83	-0.05
2,2-Dimethyloxirane	7.99	7.99	0.00
2,2-Dimethylpentane	13.72	13.69	0.03
2,2-Dimethylpentanoic acid	14.27	14.32	-0.05
2,2-Dimethylpropane	10.45	10.02	0.43
2,2-Dimethylpropylamine	11.29	11.38	-0.09
2,2-Propanedithiol	12.68	12.53	0.15
2,3,3,4-Tetramethylpentane	17.12	17.33	-0.21
2,3,3-Trimethyl-1-butene	13.46	13.59	-0.13
2,3,3-Trimethyl-1-pentene	15.32	15.43	-0.11
2,3,3-Trimethyl-2-butanol	14.00	14.23	-0.23
2,3,3-Trimethylhexane	17.30	17.34	-0.04
2,3,3-Trimethylpentane	15.36	15.51	-0.15
2,3,4,5,6-Pentafluorotoluene	12.20	12.22	-0.02
2,3,4,5,6-Pentamethylheptane	22.54	22.79	-0.25
2,3,4,5-Tetramethylhexane	18.95	19.14	-0.19
2,3,4-Trichloro-1-butene	13.71	13.81	-0.10
2,3,4-Trimethyl-2-pentene	15.38	15.49	-0.11
2,3,4-Trimethylhexane	17.29	17.32	-0.03
2,3,4-Trimethylhexanoic acid	17.90	17.95	-0.05
2,3,4-Trimethylpentane	15.41	15.48	-0.07

2,3,4-Trimethylpentanoic acid	16.07	16.12	-0.05
2,3,5-Trimethylhexane	17.27	17.32	-0.05
2,3,6-Collidine	15.46	15.46	0.00
2,3-Butandione	8.34	8.40	-0.06
2,3-Butanediol dinitrate	14.06	14.24	-0.18
2,3-Butyleneglycol	9.22	9.32	-0.10
2,3-Diaminonaphthalene	20.58	20.86	-0.28
2,3-Dibromo-1-propene	12.25	12.24	0.01
2,3-Dibromo-2-methylbutane	16.31	16.24	0.07
2,3-Dibromobutane	14.39	14.37	0.02
2,3-Dibromoheptane	19.84	19.87	-0.03
2,3-Dichloro-1,3-butadiene	11.90	11.84	0.06
2,3-Dichloro-1-propanol	10.71	10.70	0.01
2,3-Dichloro-2-methylbutane	13.91	13.86	0.05
2,3-Dichlorobutane	12.03	11.96	0.07
2,3-Dichloropentane	13.83	13.80	0.03
2,3-Dichloropropanoyl chloride	12.24	12.31	-0.07
2,3-Dichloropropene	9.95	10.08	-0.13
2,3-Dichlorotoluene	16.35	16.24	0.11
2,3-Dihydro-1,1,3-trimethyl-3-phenyl-1H-indene	30.63	30.54	0.09
2,3-Dihydro-1,4-dioxin	8.25	8.29	-0.04
2,3-Dihydro-1H-indole	14.96	15.11	-0.15
2,3-Dihydro-1-methyl-1H-indene	17.16	17.13	0.03
2,3-Dihydro-4H-1-benzothiopyran-4-one	18.77	18.71	0.06
2,3-Dihydrobenzofuran	14.33	14.17	0.16
2,3-Dihydrofuran	7.65	7.78	-0.13
2,3-Dimercapto-1-propanol	13.05	12.99	0.06
2,3-Dimethyl-1,3-butadiene	11.87	11.67	0.20
2,3-Dimethyl-1-butene	11.88	11.75	0.13
2,3-Dimethyl-1-hexene	15.52	15.42	0.10
2,3-Dimethyl-1-pentene	13.48	13.58	-0.10
2,3-Dimethyl-2-butanol	12.38	12.38	0.00
2,3-Dimethyl-2-hexene	15.50	15.51	-0.01
2,3-Dimethyl-2-iodobutane	16.93	17.10	-0.17
2,3-Dimethyl-2-norbornene	15.51	15.61	-0.10
2,3-Dimethyl-2-pentene	13.56	13.67	-0.11
2,3-Dimethyl-3-ethylpentane	17.21	17.34	-0.13
2,3-Dimethyl-3-pentanol	14.25	14.22	0.03
2,3-Dimethylbutane	11.82	11.83	-0.01
2,3-Dimethylbutanoic acid	12.42	12.46	-0.04
2,3-Dimethyldecane	22.84	22.84	0.00
2,3-Dimethyldodecane	26.52	26.51	0.01



2,3-Dimethylheptadecane	35.70	35.69	0.01
2,3-Dimethylheptane	17.31	17.33	-0.02
2,3-Dimethylheptanoic acid	17.92	17.97	-0.05
2,3-Dimethylhexadecane	33.88	33.85	0.03
2,3-Dimethylhexane	15.92	15.50	0.42
2,3-Dimethylnonadecane	39.38	39.36	0.02
2,3-Dimethylnonane	21.00	21.01	-0.01
2,3-Dimethyloctadecane	37.56	37.52	0.04
2,3-Dimethyloctane	19.13	19.17	-0.04
2,3-Dimethylpentadecane	32.03	32.02	0.01
2,3-Dimethylpentane	13.61	13.66	-0.05
2,3-Dimethylpentanoic acid	14.25	14.30	-0.05
2,3-Dimethyltetradecane	30.21	30.18	0.03
2,3-Dimethylthiophene	13.47	13.68	-0.21
2,3-Dimethyltridecane	28.37	28.35	0.02
2,3-Dimethylundecane	24.68	24.68	0.00
2,3-Heptanedione	13.85	13.91	-0.06
2,3-Lutidine	13.54	13.48	0.06
2,3-Pentadiene	10.01	10.05	-0.04
2,3-Pentanediol	11.13	11.15	-0.02
2,3-Pentanedione	10.09	10.24	-0.15
2,3-Xylidine	15.83	15.94	-0.11
2,4,4-Trimethyl-2-pentanol	16.16	16.06	0.10
2,4,4-Trimethyl-2-pentene	15.46	15.47	-0.01
2,4,4-Trimethylcyclohexanone	16.54	16.60	-0.06
2,4,4-Trimethylhexane	17.39	17.34	0.05
2,4,6,8,10,12-Hexamethylcyclohexasiloxane	34.03	33.99	0.04
2,4,6,8-Tetramethylcyclotetrasiloxane	22.65	22.66	-0.01
2,4,6-Collidine	15.31	15.46	-0.15
2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane	45.93	45.82	0.11
2,4,6-Trimethyl-3-heptene	19.16	19.12	0.04
2,4,6-Trimethylaniline	17.71	17.85	-0.14
2,4,6-Trimethylchroman	21.55	21.57	-0.02
2,4,6-Trimethyldecane	24.68	24.66	0.02
2,4,6-Trimethyldodecane	28.35	28.33	0.02
2,4,6-Trimethyleicosane	43.03	43.01	0.02
2,4,6-Trimethylheneicosane	44.86	44.85	0.01
2,4,6-Trimethylheptadecane	37.54	37.51	0.03
2,4,6-Trimethylhexadecane	35.70	35.67	0.03
2,4,6-Trimethylnonadecane	41.20	41.18	0.02
2,4,6-Trimethylnonane	22.85	22.82	0.03
2,4,6-Trimethyloctadecane	39.39	39.34	0.05

2,4,6-Trimethyloctane	21.00	20.99	0.01
2,4,6-Trimethylpentadecane	33.86	33.84	0.02
2,4,6-Trimethyltetradecane	32.03	32.00	0.03
2,4,6-Trimethyltridecane	30.18	30.17	0.01
2,4,6-Trimethylundecane	26.51	26.50	0.01
2,4-Dibromopentane	16.06	16.20	-0.14
2,4-Dibromotoluene	18.56	18.44	0.12
2,4-Dichlorotoluene	16.33	16.24	0.09
2,4-Diethylpyrrole	15.73	15.76	-0.03
2,4-Diethylpyrrolidine	15.95	15.97	-0.02
2,4-Difluoroaniline	12.00	12.05	-0.05
2,4-Dimethyl-1,3-pentadiene	13.66	13.55	0.11
2,4-Dimethyl-1-pentene	13.55	13.58	-0.03
2,4-Dimethyl-2-pentene	13.63	13.63	0.00
2,4-Dimethyl-3-ethylpentane	17.22	17.32	-0.10
2,4-Dimethyl-3-isopropylpentane	19.10	19.14	-0.04
2,4-Dimethyl-3-pentanol	14.21	14.23	-0.02
2,4-Dimethyl-3-pentanone	13.53	13.77	-0.24
2,4-Dimethylacetophenone	18.04	18.17	-0.13
2,4-Dimethyldecane	22.89	22.84	0.05
2,4-Dimethyldocosane	44.91	44.86	0.05
2,4-Dimethyldodecane	26.54	26.51	0.03
2,4-Dimethyleicosane	41.25	41.19	0.06
2,4-Dimethylheneicosane	43.07	43.03	0.04
2,4-Dimethylheptadecane	35.72	35.69	0.03
2,4-Dimethylheptane	17.45	17.33	0.12
2,4-Dimethylhexadecane	33.88	33.85	0.03
2,4-Dimethylhexane	15.49	15.50	-0.01
2,4-Dimethylhexanoic acid	16.09	16.13	-0.04
2,4-Dimethylnitrobenzene	16.75	16.97	-0.22
2,4-Dimethylnonadecane	39.43	39.36	0.07
2,4-Dimethylnonane	21.04	21.01	0.03
2,4-Dimethyloctadecane	37.57	37.52	0.05
2,4-Dimethyloctane	19.30	19.17	0.13
2,4-Dimethyloxazole	10.34	10.12	0.22
2,4-Dimethylpentadecane	32.05	32.02	0.03
2,4-Dimethylpentane	13.73	13.66	0.07
2,4-Dimethylpentanoic acid	14.25	14.30	-0.05
2,4-Dimethylpyrrole	12.11	12.09	0.02
2,4-Dimethylpyrrolidine	12.55	12.30	0.25
2,4-Dimethylquinoline	20.30	20.45	-0.15
2,4-Dimethylsulfolane	14.51	14.46	0.05

2,4-Dimethyltetradecane	30.21	30.18	0.03
2,4-Dimethylthiazole	12.68	12.44	0.24
2,4-Dimethylthiophene	13.39	13.68	-0.29
2,4-Dimethyltridecane	28.38	28.35	0.03
2,4-Dimethylundecane	24.71	24.68	0.03
2,4-Dinitroanisole	18.61	18.39	0.22
2,4-Hexanedione	12.72	12.39	0.33
2,4-Lutidine	13.44	13.48	-0.04
2,4-Pentanediol	11.18	11.15	0.03
2,4-Xylenol	14.85	15.03	-0.18
2,4-Xylidine	15.80	15.94	-0.14
2,5,5-Trimethylheptane	19.18	19.18	0.00
2,5,8,11-Tetraoxododecane	18.22	18.19	0.03
2,5-Aldehydine	15.28	15.32	-0.04
2,5-Dibromoheptane	19.89	19.87	0.02
2,5-Dibromooctane	21.82	21.71	0.11
2,5-Dibromothiophene	15.91	15.90	0.01
2,5-Dibromotoluene	18.65	18.44	0.21
2',5'-Dichloroacetophenone	18.33	18.18	0.15
2,5-Dichlorostyrene	18.32	17.95	0.37
2,5-Dichlorothiophene	13.65	13.57	0.08
2,5-Dichlorotoluene	16.10	16.24	-0.14
2,5-Diethylpyrrole	15.57	15.73	-0.16
2,5-Dihydro-1H-pyrrole	8.35	8.60	-0.25
2,5-Dihydro-2,5-dimethoxyfuran	12.52	12.79	-0.27
2',5'-Dimethoxyacetophenone	19.80	19.53	0.27
2,5-Dimethyl-1,5-hexadiene	15.50	15.34	0.16
2,5-Dimethyl-2,5-hexanediamine	17.97	18.19	-0.22
2,5-Dimethyl-2-hexene	15.48	15.46	0.02
2,5-Dimethyl-4-hendecene	24.55	24.64	-0.09
2,5-Dimethyl-5-undecanol	25.16	25.23	-0.07
2,5-Dimethylacetophenone	18.19	18.17	0.02
2,5-Dimethylbenzoxazole	16.85	17.00	-0.15
2,5-Dimethylfuran	11.22	11.29	-0.07
2,5-Dimethylheptane	17.25	17.33	-0.08
2,5-Dimethylhexane	15.64	15.50	0.14
2,5-Dimethyloctane	19.29	19.17	0.12
2,5-Dimethyloxazole	10.16	10.17	-0.01
2,5-Dimethylpyrazine	12.71	12.64	0.07
2,5-Dimethylpyrrole	11.93	12.05	-0.12
2,5-Dimethyltetrahydrofuran	11.40	11.69	-0.29
2,5-Dimethylthiophene	13.57	13.79	-0.22

2,5-Dimethylundecane	24.61	24.68	-0.07
2,5-Dioxaheptane	11.42	11.35	0.07
2,5-Dipropyl-3-ethylthiophane	25.22	25.14	0.08
2,5-Dipropyl-3-methylthiophane	23.24	23.30	-0.06
2,5-Dipropylpyrrole	19.37	19.40	-0.03
2,5-Di-t-butylfuran	22.42	22.29	0.13
2,5-Hexanediol	13.04	12.99	0.05
2,5-Lutidine	13.45	13.48	-0.03
2,5-Xylidine	15.84	15.94	-0.10
2,6-Dichloroaniline	15.98	15.95	0.03
2,6-Dichloroanisole	17.13	16.92	0.21
2,6-Dichlorotoluene	16.05	16.24	-0.19
2,6-Difluoropyridine	9.43	9.30	0.13
2,6-Diisopropylaniline	23.21	23.25	-0.04
2,6-Diisopropylphenol	22.28	22.34	-0.06
2,6-Dimethyl-2-heptanol	17.83	17.89	-0.06
2,6-Dimethyl-2-heptene	17.33	17.30	0.03
2,6-Dimethyl-4-ethylpyridine	17.24	17.29	-0.05
2,6-Dimethyl-4-heptanol	17.99	17.90	0.09
2,6-Dimethylanisole	16.66	16.91	-0.25
2,6-Dimethylchroman	19.87	19.75	0.12
2,6-Dimethylcyclohexanone	14.42	14.76	-0.34
2,6-Dimethylheptan-4-one	17.39	17.44	-0.05
2,6-Dimethylheptane	17.43	17.33	0.10
2,6-Dimethylmorpholine	13.05	12.96	0.09
2,6-Dimethyloctane	19.09	19.17	-0.08
2,6-Dimethylpentamethylene sulfide	16.06	15.98	0.08
2,6-Dimethylpiperidine	14.43	14.13	0.30
2,6-Dinitrotoluene	17.51	17.71	-0.20
2,6-Di-t-butyl-p-cresol	28.06	27.93	0.13
2,6-Di-t-butylpyridine	24.97	24.55	0.42
2,6-Lutidine	13.43	13.55	-0.12
2,6-Nonadien-1-ol	17.69	17.77	-0.08
2,6-Xylidine	15.80	15.94	-0.14
2,7-Dimethyloctane	19.34	19.17	0.17
2,9-Dimethyl-5,6-diisoamyldecane	40.98	41.13	-0.15
2-Acetoxy-4-oxa-6-oxononane	20.60	20.68	-0.08
2-Acetoxyanisole	17.46	17.54	-0.08
2-Acetoxyethylphosphine	12.77	12.84	-0.07
2-Acetylfuran	11.73	11.36	0.37
2-Acetylthiophene	13.98	13.76	0.22
2-Allylphenol	16.38	16.67	-0.29

2-Amino-1-butanol	10.34	10.08	0.26
2-Aminoisobutanol	10.15	10.08	0.07
2-Anisaldehyde	15.41	15.21	0.20
2-Benzylpyridine	20.88	21.31	-0.43
2-Benzyltetrahydropyran	21.31	21.42	-0.11
2-Benzylthiophene	21.23	21.55	-0.32
2-Bromo-1,1,1-trifluoroethane	7.43	7.70	-0.27
2-Bromo-1,1-diethoxyethane	16.01	16.20	-0.19
2-Bromo-1,1-dimethoxyethane	12.47	12.51	-0.04
2-Bromo-1,3,5-trimethylbenzene	19.09	19.24	-0.15
2-Bromo-1,3-butadiene	11.08	10.88	0.20
2-Bromo-1-butene	10.94	11.00	-0.06
2-Bromo-1-chloro-3,3-dimethylbutane	17.27	16.84	0.43
2-Bromo-1-chloropropane	11.52	11.34	0.18
2-Bromo-1-phenyl-1-propanone	19.44	19.28	0.16
2-Bromo-2-chloro-1,1,1-trifluoroethane	9.53	9.58	-0.05
2-Bromo-2-chloro-4,4-dimethylpentane	19.02	18.85	0.17
2-Bromo-2-chlorobutane	13.32	13.35	-0.03
2-Bromo-2-chloropropane	11.38	11.52	-0.14
2-Bromo-2-methylbutane	13.24	13.16	0.08
2-Bromo-2-methylpropane	11.46	11.32	0.14
2-Bromo-3,3-difluoro-2-propen-1-ol	9.66	9.57	0.09
2-Bromo-3-methyl-1-butene	12.89	12.82	0.07
2-Bromo-4-methylaniline	16.71	17.04	-0.33
2-Bromo-4-methylphenol	15.94	16.13	-0.19
2-Bromo-4-phenyl-1-butene	20.50	20.74	-0.24
2-Bromo-5-chlorothiophene	14.70	14.73	-0.03
2-Bromoallyl alcohol	9.85	9.73	0.12
2-Bromoaniline	15.01	15.13	-0.12
2-Bromoanisole	16.26	16.11	0.15
2-Bromobutane	11.30	11.28	0.02
2-Bromobutanoic acid	11.83	11.91	-0.08
2-Bromodecanoic acid	22.87	22.92	-0.05
2-Bromododecanoic acid	26.34	26.59	-0.25
2-Bromoethanesulfonylchloride	13.10	13.07	0.03
2-Bromoethanol	8.15	8.15	0.00
2-Bromohexane	14.81	14.95	-0.14
2-Bromiodobenzene	18.38	18.50	-0.12
2-Bromoisobutyronitrile	11.14	11.24	-0.10
2-Bromo-N,N-dimethylaniline	18.93	19.08	-0.15
2-Bromonaphthalene	20.52	20.64	-0.12
2-Bromooctane	18.70	18.62	0.08

2-Bromopentane	13.10	13.11	-0.01
2-Bromopropane	9.49	9.44	0.05
2-Bromopropanoic acid	10.05	10.08	-0.03
2-Bromopropanoyl chloride	11.33	11.61	-0.28
2-Bromopropene	9.17	9.17	0.00
2-Bromothiophene	12.89	12.87	0.02
2-Bromotoluene	15.32	15.43	-0.11
2-Butanethiol	11.28	11.23	0.05
2-Butanol	8.79	8.75	0.04
2-Butanone	8.25	8.30	-0.05
2-Butanone ketazine	17.95	17.96	-0.01
2-Butanone O-ethyloxime	13.75	13.77	-0.02
2-Butanone O-propyloxime	15.50	15.60	-0.10
2-Buten-1-ol	8.65	8.67	-0.02
2-Butenoyl chloride	10.41	10.27	0.14
2-Butoxy-2-bora-1,3-dioxacyclopentane	14.72	14.51	0.21
2-Butoxy-4,4-bis(ethylthio)-butane	29.86	29.80	0.06
2-Butoxy-4-methyl-1,3,2-dioxaphospholane	18.02	18.09	-0.07
2-Butoxyphenol	19.25	19.32	-0.07
2-Butoxypyridine	17.86	17.93	-0.07
2-Butoxyvinyl bis(diethylamino) phosphorus oxide	33.13	33.18	-0.05
2-Butoxyvinyl bis(dimethylamino) phosphorus oxide	25.94	25.90	0.04
2-Butoxyvinyl diethoxy phosphorus oxide	24.47	24.61	-0.14
2-Butoxyvinyl dimethoxy phosphorus oxide	21.24	20.91	0.33
2-Butyl-2-ethyl-1,3-propanediol	18.72	18.48	0.24
2-Butyl-3-ethyl-5-propylthiophane	26.88	26.98	-0.10
2-Butylamine	9.55	9.52	0.03
2-Butylbiphenyl	27.88	27.73	0.15
2-Butylnaphthalene	25.12	25.04	0.08
2-Butylphenol	18.51	18.63	-0.12
2-Butylsilane	12.30	12.32	-0.02
2-Butyltetrahydropyran	17.18	17.19	-0.01
2-Butylthiophene	17.15	17.32	-0.17
2-Butylthiovinyl diallyloxy phosphorus oxide	30.08	30.52	-0.44
2-Butylthiovinyl dibutoxy phosphorus oxide	34.22	34.44	-0.22
2-Butylthiovinyl dichloro phosphorus oxide	22.93	22.81	0.12
2-Butyn-1-al	7.77	7.80	-0.03
2-Butyn-1-ol	8.02	8.15	-0.13
2-Butyne	7.39	7.60	-0.21
2-Butynedinitrile	7.30	7.43	-0.13
2-Butyrylthiophene	17.60	17.43	0.17
2-Chloro-1,1,1-trifluoroethane	6.50	6.53	-0.03

2-Chloro-1,1-diethoxyethane	14.94	15.04	-0.10
2-Chloro-1,1-difluoro-4-iodo-1-butene	14.82	14.96	-0.14
2-Chloro-1,1-dimethoxyethane	11.58	11.34	0.24
2-Chloro-1,3-propanediol	9.47	9.36	0.11
2-Chloro-1-butanol	10.70	10.64	0.06
2-Chloro-1-butene	9.90	10.02	-0.12
2-Chloro-1-ethylbenzene	16.08	16.17	-0.09
2-Chloro-1-propanol	8.94	8.80	0.14
2-Chloro-1-trichloromethoxybenzene	20.82	20.77	0.05
2-Chloro-1-trifluoromethoxybenzene	14.92	14.84	0.08
2-Chloro-1-trifluoromethylbenzene	14.11	14.44	-0.33
2-Chloro-2,4,4-trimethylpentane	17.44	17.47	-0.03
2-Chloro-2-methylbutane	11.98	11.97	0.01
2-Chloro-2-methylpropanal	10.06	10.34	-0.28
2-Chloro-2-methylpropane	10.23	10.14	0.09
2-Chloro-2-propenenitrile	8.16	8.10	0.06
2-Chloro-3,3-difluoro-2-propen-1-ol	8.71	8.58	0.13
2-Chloro-4-methylaniline	16.11	15.94	0.17
2-Chloro-4-methylpentane	13.80	13.73	0.07
2-Chloro-5-(trifluoromethyl)aniline	15.90	16.05	-0.15
2-Chloro-6-phenylphenol	23.09	22.93	0.16
2-Chloroacetophenone	16.01	16.27	-0.26
2-Chloroacrolein	8.24	8.39	-0.15
2-Chloroacrylaldehyde	8.24	8.34	-0.10
2-Chloroallyl alcohol	8.63	8.74	-0.11
2-Chloroaniline	14.18	14.04	0.14
2-Chloroanisole	15.07	15.01	0.06
2-Chlorobenzaldehyde	14.56	14.54	0.02
2-Chlorobenzyl chloride	16.09	16.23	-0.14
2-Chlorobutane	10.12	10.08	0.04
2-Chlorobutanoic acid	10.88	10.71	0.17
2-Chlorobutanoic acid methylester	12.33	12.59	-0.26
2-Chlorocrotonaldehyde	10.29	10.27	0.02
2-Chlorocyclohexanone	12.93	13.01	-0.08
2-Chlorocyclopentanone	11.17	11.17	0.00
2-Chloroethanesulfonyl chloride	12.05	11.91	0.14
2-Chloroethanol	7.02	6.98	0.04
2-Chloroethyl acetoacetate	14.35	14.56	-0.21
2-Chloroethyl chloroformate	10.96	10.94	0.02
2-Chloroethyl crotonate	14.42	14.38	0.04
2-Chloroethyl ethyl ether	10.81	10.76	0.05
2-Chloroethyl vinyl ether	10.56	10.48	0.08

2-Chloroethylsulfonyl fluoride	10.08	10.24	-0.16
2-Chloroethylthiobenzene	19.43	19.45	-0.02
2-Chloroheptane	15.65	15.58	0.07
2-Chlorohexane	13.75	13.75	0.00
2-Chloriodobenzene	17.30	17.41	-0.11
2-Chloroisopropylacetate	12.76	12.79	-0.03
2-Chloro-N-(2-chloroethyl)-N-ethylethanamine	17.17	17.18	-0.01
2-Chloro-N,N-diallylacetamide	18.39	18.68	-0.29
2-Chloro-N,N-dimethylaniline	17.96	17.98	-0.02
2-Chloronaphthalene	19.59	19.54	0.05
2-Chlorooctane	17.49	17.42	0.07
2-Chloro-p-cresol	14.58	15.03	-0.45
2-Chloropentane	11.96	11.91	0.05
2-Chloropentanoic acid	12.69	12.55	0.14
2-Chlorophenol	12.89	13.12	-0.23
2-Chloropropanal	8.03	8.45	-0.42
2-Chloropropane	8.32	8.24	0.08
2-Chloropropanoic acid	8.97	8.88	0.09
2-Chloropropene	8.11	8.18	-0.07
2-Chloropyridine	11.57	11.60	-0.03
2-Chloroquinoline	18.61	18.57	0.04
2-Chlorostyrene	16.26	16.04	0.22
2-Chlorothiophene	11.62	11.70	-0.08
2-Chlorotoluene	14.25	14.33	-0.08
2-Cyanobutane	9.95	9.93	0.02
2-Cyanoethanol	6.92	6.83	0.09
2-Cyanopropan-2-ol	8.59	8.65	-0.06
2-Cyclohexen-1-ol	11.12	11.50	-0.38
2-Cyclohexene-1-one	11.42	11.04	0.38
2-Cyclohexyl-2-methylpentadecane	40.32	40.35	-0.03
2-Cyclohexylcyclohexanone	21.22	21.25	-0.03
2-Cyclohexyltetradecane	36.80	36.67	0.13
2-Cyclohexyltetrahydropyran	20.07	20.00	0.07
2-Cyclohexylthiacyclohexane	22.38	22.46	-0.08
2-Cyclopenten-1-one	9.06	9.20	-0.14
2-Cyclopentylidenecyclopentanone	17.83	17.59	0.24
2-Cyclopentylthiacyclohexane	20.70	20.62	0.08
2-Decanol	19.75	19.76	-0.01
2-Decanone	19.23	19.31	-0.08
2-Decyn-1-ol	18.99	19.17	-0.18
2-Diethylaminoethanol	13.76	13.93	-0.17
2-Diethylaminoethylamine	14.49	14.73	-0.24



2-Dodecanol	23.49	23.44	0.05
2-Dodecanone	23.17	22.98	0.19
2-Ethoxy-1,2-diphenylethanone	28.48	28.44	0.04
2-Ethoxy-3,4-dihydro-2H-pyran	13.85	13.89	-0.04
2-Ethoxy-4-methyl-1,3,2-dioxaphospholane	14.36	14.42	-0.06
2-Ethoxyethanamine	10.29	10.22	0.07
2-Ethoxyethanol	9.53	9.42	0.11
2-Ethoxyethyl acrylate	14.94	14.94	0.00
2-Ethoxyethylacetate	13.20	13.22	-0.02
2-Ethoxymethylthiophene	15.93	16.15	-0.22
2-Ethoxynaphthalene	21.88	22.06	-0.18
2-Ethoxythiophene	14.16	14.10	0.06
2-Ethoxyvinyl bis(dibutylamino) phosphorus oxide	43.75	44.19	-0.44
2-Ethoxyvinyl bis(dimethylamino) phosphorus oxide	22.25	22.23	0.02
2-Ethyl-1,3,5-trimethylbenzene	19.82	19.97	-0.15
2-Ethyl-1,3-butadiene	11.80	11.64	0.16
2-Ethyl-1-butanol	12.36	12.40	-0.04
2-Ethyl-1-butene	11.65	11.77	-0.12
2-Ethyl-1-hexanol	16.03	16.07	-0.04
2-Ethyl-1-pentene	13.48	13.60	-0.12
2-Ethyl-2 methyl-5-propylthiophane	21.62	21.64	-0.02
2-Ethyl-2-methyl-5-propyltetrahydrofuran	19.06	19.01	0.05
2-Ethyl-3-methyl-1-butene	13.49	13.58	-0.09
2-Ethyl-3-methyl-1-pentene	15.34	15.42	-0.08
2-Ethyl-3-methyl-5-propylthiophane	21.62	21.47	0.15
2-Ethyl-3-propyl-1,4-dioxane	17.76	17.87	-0.11
2-Ethyl-4-isopropylpyrrolidine	17.77	17.79	-0.02
2-Ethyl-4-methylpyrrole	13.85	13.93	-0.08
2-Ethyl-4-methylpyrrolidine	14.33	14.14	0.19
2-Ethyl-4-oxo-1-heptanol	17.88	18.02	-0.14
2-Ethyl-5-methylthiophane	16.01	15.98	0.03
2-Ethyl-5-methylthiophane sulfone	16.18	16.31	-0.13
2-Ethyl-5-propylpyrrole	17.53	17.56	-0.03
2-Ethyl-5-propylthiophane	19.61	19.65	-0.04
2-Ethyl-5-propylthiophane sulfone	19.70	19.98	-0.28
2-Ethyl-6-methylaniline	17.71	17.77	-0.06
2-Ethylaniline	15.76	15.87	-0.11
2-Ethylbutanoic acid	12.43	12.48	-0.05
2-Ethylbutyl acetate	16.15	16.21	-0.06
2-Ethylbutyryl chloride	13.84	14.01	-0.17
2-Ethylfuran	11.14	11.25	-0.11
2-Ethylheptanoic acid	17.94	17.98	-0.04

2-Ethylhexanal	15.72	15.72	0.00
2-Ethylhexanoic acid	16.16	16.15	0.01
2-Ethylhexanoyl chloride	17.87	17.68	0.19
2-Ethylhexyl acetate	19.84	19.88	-0.04
2-Ethylhexyl acrylate	21.58	21.59	-0.01
2-Ethylhexyl methacrylate	23.36	23.45	-0.09
2-Ethyl-m-xylene	17.97	18.07	-0.10
2-Ethyl-naphthalene	21.36	21.37	-0.01
2-Ethyl-nitrobenzene	16.66	16.90	-0.24
2-Ethyl-nonanoic acid	21.61	21.66	-0.05
2-Ethyl-octanoic acid	19.77	19.82	-0.05
2-Ethyl-pentamethylene sulfide	15.99	15.98	0.01
2-Ethyl-pentanoic acid	14.25	14.31	-0.06
2-Ethyl-p-xylene	18.05	18.07	-0.02
2-Ethyl-pyridine	13.07	13.41	-0.34
2-Ethylstyrene	18.18	17.87	0.31
2-Ethyl-tetrahydrofuran	11.59	11.69	-0.10
2-Ethyl-tetrahydropyran	13.51	13.52	-0.01
2-Ethylthioethanol	11.90	11.89	0.01
2-Ethylthiophene	13.45	13.65	-0.20
2-Ethylthiovinyl bis(ethoxyethoxy) phosphorus oxide	32.18	32.10	0.08
2-Ethylthiovinyl bis(methoxyethoxy) phosphorus oxide	28.43	28.41	0.02
2-Ethylthiovinyl diallyloxy phosphorus oxide	26.56	26.85	-0.29
2-Ethylthiovinyl dibutoxy phosphorus oxide	31.09	30.76	0.33
2-Ethylthiovinyl dichloro phosphorus oxide	19.19	19.14	0.05
2-Ethylthiovinyl dihexoxy phosphorus oxide	37.72	38.11	-0.39
2-Ethylthiovinyl dipropoxy phosphorus oxide	26.90	27.09	-0.19
2-Ethyltoluene	16.03	16.16	-0.13
2-Fluoro-1,1,2-trichloroethane	10.25	10.29	-0.04
2-Fluoro-1,3-butadiene	8.23	7.90	0.33
2-Fluoro-1-phenylethanone	14.45	14.33	0.12
2-Fluoro-2-methylbutane	9.88	9.97	-0.09
2-Fluoro-4-methylpyridine	11.35	11.36	-0.01
2-Fluoro-6-methylpyridine	11.36	11.42	-0.06
2-Fluoroaniline	12.04	12.09	-0.05
2-Fluoroanisole	12.73	13.06	-0.33
2-Fluorobenzaldehyde	12.77	12.59	0.18
2-Fluorobenzotrifluoride	12.30	12.49	-0.19
2-Fluorobenzoyl chloride	14.77	14.54	0.23
2-Fluoroethanol	5.14	5.05	0.09
2-Fluoronitrobenzene	13.39	13.12	0.27

2-Fluorophenylethylether	14.85	14.90	-0.05
2-Fluoropyridine	9.30	9.45	-0.15
2-Fluorotoluene	12.14	12.38	-0.24
2-Formylnaphthalene	20.21	19.74	0.47
2-Furancarbonitrile	9.68	9.33	0.35
2-Furanmethanethiol	12.41	12.45	-0.04
2-Furfurylamine	10.56	10.77	-0.21
2-Heptanamine	15.08	15.03	0.05
2-Heptanol	14.30	14.26	0.04
2-Heptanone	13.79	13.80	-0.01
2-Heptanoylthiophene	23.17	22.93	0.24
2-Heptenal	13.75	13.82	-0.07
2-Heptyl bromide	16.93	16.78	0.15
2-Heptylnaphthalene	30.69	30.55	0.14
2-Heptylthiophene	22.69	22.82	-0.13
2-Heptyne	13.05	13.10	-0.05
2-Hexanethiol	14.95	14.90	0.05
2-Hexanol	12.42	12.42	0.00
2-Hexanoylthiophene	21.33	21.10	0.23
2-Hexenoic acid	12.50	12.42	0.08
2-Hexoxy-4-methyl-1,3,2-dioxaphospholane	21.69	21.76	-0.07
2-Hexylnaphthalene	28.84	28.72	0.12
2-Hexylthiacyclohexane	23.39	23.32	0.07
2-Hexylthiophene	20.86	20.99	-0.13
2-Hexyne	11.12	11.27	-0.15
2-Hydroxy-1-phenyl-1-propanone	16.74	16.76	-0.02
2-Hydroxy-2-dibutylphosphonato-3-butanone	27.95	28.01	-0.06
2-Hydroxy-2-diethylphosphonato-3-butanone	20.73	20.67	0.06
2-Hydroxy-2-dimethylphosphonato-3-butanone	16.96	16.97	-0.01
2-Hydroxy-5-methylbenzaldehyde	15.69	15.23	0.46
2-Hydroxyacetophenone	15.40	15.06	0.34
2-Hydroxybenzaldehyde	13.68	13.33	0.35
2-Hydroxybenzonitrile	13.35	13.04	0.31
2-Hydroxybicyclopentyl	18.02	18.04	-0.02
2-Hydroxyethylammonium acetate	11.62	11.49	0.13
2-hydroxyethylammonium butanoate	15.27	15.16	0.11
2-Hydroxyethylammonium formate	9.85	9.79	0.06
2-Hydroxyethylammonium hexanoate	18.95	18.83	0.12
2-Hydroxyethylammonium lactate	13.75	13.89	-0.14
2-Hydroxyethylammonium pentanoate	17.09	17.00	0.09
2-Hydroxyethylammonium propionate	13.20	13.33	-0.13
2-Hydroxyethylmethacrylate	12.89	13.02	-0.13

2-Hydroxyethylphosphine	8.99	9.04	-0.05
2-Hydroxythiophene	10.29	10.37	-0.08
2-Indanone	15.30	15.42	-0.12
2-Iodo-2-methylbutane	15.41	15.28	0.13
2-Iodo-2-methylpropane	13.47	13.45	0.02
2-Iodoacetophenone	19.57	19.34	0.23
2-Iodobutane	13.45	13.43	0.02
2-Iodoethanol	10.20	10.18	0.02
2-Iodonaphthalene	22.95	22.61	0.34
2-Iodooctane	20.75	20.77	-0.02
2-Iodopropane	11.69	11.59	0.10
2-Iodotoluene	17.45	17.40	0.05
2-Isoamyoxyvinyl bis(dibutylamino) phosphorus oxide	49.50	49.68	-0.18
2-Isobutylfuran	14.81	14.90	-0.09
2-Isobutyltetrahydrofuran	15.36	15.34	0.02
2-Isobutyrylthiophene	17.67	17.41	0.26
2-Isopropoxyethanol	11.32	11.26	0.06
2-Isopropoxyvinyl bis(dimethylamino) phosphorus oxide	24.11	24.07	0.04
2-Isopropyl-5-methylphenol	18.75	18.68	0.07
2-Isopropylnaphthalene	23.19	23.19	0.00
2-Isopropyl-p-cresol	18.49	18.68	-0.19
2-Isopropyltetrahydropyran	15.31	15.34	-0.03
2-Isopropyltoluene	17.87	17.98	-0.11
2-Mercaptoethanol	8.17	8.12	0.05
2-Methoxy-1,1'-biphenyl	23.22	22.90	0.32
2-Methoxy-1,3-butadiene	10.71	10.33	0.38
2-Methoxy-1-phenylethanone	17.12	16.85	0.27
2-Methoxy-1-propanol	9.37	9.41	-0.04
2-Methoxy-4-methyl-1,3,2-dioxaphospholane	12.49	12.57	-0.08
2-Methoxyaniline	14.68	14.71	-0.03
2-Methoxybenzenemethanamine	16.42	16.36	0.06
2-Methoxyethyl acetate	11.27	11.38	-0.11
2-Methoxymethylthiophene	14.04	14.31	-0.27
2-Methoxynitrobenzene	15.68	15.74	-0.06
2-Methoxy-p-cresol	15.53	15.71	-0.18
2-Methoxyphenol	13.74	13.80	-0.06
2-Methoxypyridine	12.25	12.41	-0.16
2-Methoxystyrene	16.58	16.72	-0.14
2-Methoxythiophene	12.28	12.26	0.02
2-Methyl-1,2-propanediamine	10.97	10.88	0.09

2-Methyl-1,2-propanediol	9.30	9.29	0.01
2-Methyl-1,3-cyclohexadiene	12.52	12.72	-0.20
2-Methyl-1,3-dioxolane	8.70	8.62	0.08
2-Methyl-1,3-propanediol	9.37	9.29	0.08
2-Methyl-1,4-dibromobutane	16.00	16.15	-0.15
2-Methyl-1,5-dibromopentane	17.89	17.98	-0.09
2-Methyl-1,5-hexadiene	13.44	13.48	-0.04
2-Methyl-1,5-pentanediol	13.02	12.96	0.06
2-Methyl-1-butanethiol	13.03	13.05	-0.02
2-Methyl-1-butanol	10.60	10.57	0.03
2-Methyl-1-butyl acetate	14.44	14.37	0.07
2-Methyl-1-heptanol	16.42	16.07	0.35
2-Methyl-1-heptene	15.59	15.44	0.15
2-Methyl-1-hexanol	14.19	14.24	-0.05
2-Methyl-1-hexene	13.58	13.60	-0.02
2-Methyl-1H-indene	17.26	17.10	0.16
2-Methyl-1-nonene	19.15	19.11	0.04
2-Methyl-1-octene	17.19	17.27	-0.08
2-Methyl-1-pentanol	12.36	12.40	-0.04
2-Methyl-1-pentene	11.69	11.77	-0.08
2-Methyl-1-phenyl-1-propanone	18.03	18.02	0.01
2-Methyl-1-propanethiol	11.25	11.21	0.04
2-Methyl-1-propanol	8.80	8.73	0.07
2-Methyl-1-undecanol	23.37	23.42	-0.05
2-Methyl-2-butanamine	11.34	11.36	-0.02
2-Methyl-2-butanol	10.58	10.56	0.02
2-Methyl-2-chloropentadecane	32.24	32.16	0.08
2-Methyl-2-cyclohexen-1-one	12.91	12.90	0.01
2-Methyl-2-cyclopenten-1-one	10.96	11.07	-0.11
2-Methyl-2-heptanol	16.21	16.07	0.14
2-Methyl-2-heptene	15.53	15.48	0.05
2-Methyl-2-hexanol	14.28	14.23	0.05
2-Methyl-2-hexene	13.72	13.64	0.08
2-Methyl-2-octanol	17.92	17.91	0.01
2-Methyl-2-pentadecanol	30.84	30.75	0.09
2-Methyl-2-pentanol	12.02	12.40	-0.38
2-Methyl-2-pentenal	12.16	12.01	0.15
2-Methyl-2-pentene	11.80	11.81	-0.01
2-Methyl-2-phenyloxirane	15.89	15.89	0.00
2-Methyl-2-phenylpentadecane	39.74	39.94	-0.20
2-Methyl-2-propanol	8.79	8.73	0.06
2-Methyl-2-propenol	8.59	8.65	-0.06

2-Methyl-3-amino-4-methoxymethyl-5-aminomethylpyridine	21.09	20.85	0.24
2-Methyl-3-butyn-2-ol	9.81	9.76	0.05
2-Methyl-3-heptanol	16.08	16.08	0.00
2-Methyl-3-hexanone	13.69	13.79	-0.10
2-Methyl-3-hexyne	13.06	13.09	-0.03
2-Methyl-3-pentanol	12.37	12.41	-0.04
2-Methyl-3-pentenoic acid	12.35	12.40	-0.05
2-Methyl-4,6-dicrotylphenol	27.43	27.79	-0.36
2-Methyl-4-crotylphenol	20.32	20.45	-0.13
2-Methyl-4-ethylpyrrolidine	14.33	14.14	0.19
2-Methyl-4-heptanol	16.07	16.08	-0.01
2-Methyl-4-heptanone	15.50	15.62	-0.12
2-Methyl-4-hexanone	13.72	13.79	-0.07
2-Methyl-4-isopropylpyrrolidine	15.95	15.96	-0.01
2-Methyl-4-oxo-1-heptanol	16.02	16.18	-0.16
2-Methyl-5-ethylpyrrole	13.83	13.89	-0.06
2-Methyl-5-phenylpyridine	21.83	21.38	0.45
2-Methyl-5-propylpyrrole	15.61	15.73	-0.12
2-Methyl-5-propylthiophane	17.86	17.81	0.05
2-Methyl-5-propylthiophane sulfone	18.03	18.15	-0.12
2-Methyl-5-undecanol	23.41	23.42	-0.01
2-Methyl-6-propyldioxane	16.01	16.03	-0.02
2-Methylacrylonitrile	8.06	8.01	0.05
2-Methylaminoethanol	8.35	8.26	0.09
2-Methylanisole	14.85	15.00	-0.15
2-Methylbenzaldehyde	14.61	14.53	0.08
2-Methylbenzeneethanol	16.56	16.72	-0.16
2-Methylbenzenemethanamine	15.52	15.69	-0.17
2-Methylbenzimidazole	16.42	16.41	0.01
2-Methylbenzo[b]furane	15.82	15.80	0.02
2-Methylbenzoic acid	15.25	14.96	0.29
2-Methylbenzothiazole	17.41	17.53	-0.12
2-Methylbenzoxazole	14.99	15.09	-0.10
2-Methylbutanoyl chloride	12.12	12.17	-0.05
2-Methylbutyl acrylate	16.10	16.09	0.01
2-Methylbutyric acid	10.63	10.64	-0.01
2-Methylcyclohexanone	12.88	12.94	-0.06
2-Methylcyclohexyl acrylate	18.99	18.91	0.08
2-Methylcyclopentanone	11.14	11.10	0.04
2-Methyldecane	21.08	21.02	0.06
2-Methyldecanoic acid	21.61	21.66	-0.05

2-Methyldiphenylmethane	23.87	24.06	-0.19
2-Methyldodecane	24.70	24.69	0.01
2-Methylenecyclohexanol	13.33	13.32	0.01
2-Methylfuran	9.28	9.41	-0.13
2-Methylheptadecane	33.91	33.87	0.04
2-Methylheptane	15.55	15.52	0.03
2-Methylheptanoic acid	16.10	16.15	-0.05
2-Methylheptyl acetate	19.81	19.88	-0.07
2-Methylhexadecane	32.11	32.03	0.08
2-Methylhexane	13.71	13.68	0.03
2-Methylhexanoic acid	14.21	14.31	-0.10
2-Methylindole	17.35	16.85	0.50
2-Methylnaphthalene	19.21	19.54	-0.33
2-Methylnonadecane	37.58	37.54	0.04
2-Methylnonane	19.19	19.19	0.00
2-Methylnonanoic acid	19.77	19.82	-0.05
2-Methyloctadecane	35.77	35.70	0.07
2-Methyloctane	17.49	17.35	0.14
2-Methyloctanoic acid	17.94	17.98	-0.04
2-Methyloxazoline	8.74	9.04	-0.30
2-Methyloxetane	8.03	8.02	0.01
2-Methylpentadecane	30.25	30.20	0.05
2-Methylpentane	12.26	11.84	0.42
2-Methylpentanedinitrile	11.75	11.68	0.07
2-Methylpentanoic acid	12.44	12.48	-0.04
2-Methylpiperidine	12.42	12.32	0.10
2-Methylpropanal	8.25	8.38	-0.13
2-Methylpropanoic acid	8.94	8.81	0.13
2-Methylpropenoic acid	8.71	8.73	-0.02
2-Methylpropylamine	9.68	9.53	0.15
2-Methylpyrazine	10.73	10.66	0.07
2-Methylpyrrole	10.07	10.23	-0.16
2-Methylquinoline	18.60	18.54	0.06
2-Methylstyrene	16.28	16.04	0.24
2-Methyltetradecane	28.43	28.36	0.07
2-Methyltetradecane-2-ol	28.98	28.92	0.06
2-Methyltetrahydrofuran	9.80	9.85	-0.05
2-Methyltetrahydropyran	11.70	11.69	0.01
2-Methylthiophene	11.61	11.81	-0.20
2-Methyltridecane	26.56	26.53	0.03
2-Methylundecanal	22.78	23.06	-0.28
2-Methylundecane	22.90	22.86	0.04

2-Naphthyl chlorofluorophosphate	23.06	23.09	-0.03
2-Naphthylamine	19.49	19.25	0.24
2-n-Hexoxyethanol	16.84	16.76	0.08
2-Nitro-1-butanol	10.96	10.92	0.04
2-Nitro-1-propanol	9.23	9.09	0.14
2-Nitro-1-propene	8.54	8.28	0.26
2-Nitroacetophenone	16.78	17.01	-0.23
2-Nitrobutane	10.36	10.36	0.00
2-Nitroethanol	7.55	7.35	0.20
2-Nitroethylbenzene	16.72	16.53	0.19
2-Nitrophenol	14.02	13.86	0.16
2-Nitropropane	8.56	8.53	0.03
2-Nitrotoluene	14.80	15.06	-0.26
2-Nonanol	17.62	17.93	-0.31
2-Nonanone	17.42	17.47	-0.05
2-Nonenal	17.76	17.49	0.27
2-Nonynoic acid	17.17	17.41	-0.24
2-Octanamine	16.85	16.86	-0.01
2-Octanol	15.96	16.09	-0.13
2-Octanone	15.52	15.64	-0.12
2-Octen-1-ol	15.97	16.01	-0.04
2-Octylnaphthalene	32.53	32.39	0.14
2-Octyn-1-ol	15.43	15.50	-0.07
2-Octyne	14.79	14.94	-0.15
2-Octynoic acid	15.33	15.57	-0.24
2-Oxetanone	6.18	6.20	-0.02
2-Oxiranylmethanol	6.79	6.74	0.05
2-Pentanol	10.59	10.59	0.00
2-Pentanone ketazine	21.66	21.63	0.03
2-Pentanone O-ethyloxime	15.60	15.60	0.00
2-Pentanone O-propyloxime	17.39	17.44	-0.05
2-Pentanone oxime	11.73	11.73	0.00
2-Pentanoylthiophene	19.45	19.26	0.19
2-Pentoxy-4-methyl-1,3,2-dioxaphospholane	19.64	19.93	-0.29
2-Pentylnaphthalene	26.99	26.88	0.11
2-Pentyloxytrimethylsilane	19.72	19.65	0.07
2-Pentyltetrahydrofuran	17.15	17.19	-0.04
2-Pentylthiophene	19.03	19.15	-0.12
2-Pentyn-1-ol	9.89	9.99	-0.10
2-Pentyne	9.36	9.43	-0.07
2-Phenoxy-1-propanol	17.36	17.34	0.02
2-Phenoxyethanol	15.45	15.50	-0.05



2-Phenoxypropanoyl chloride	18.69	18.95	-0.26
2-Phenoxyvinyl bis(dibutylamino) phosphorus oxide	50.34	50.27	0.07
2-Phenoxyvinyl bis(diethylamino) phosphorus oxide	35.96	35.59	0.37
2-Phenyl-1,3-butadiene	17.74	17.71	0.03
2-Phenyl-1-propanol	16.78	16.63	0.15
2-Phenyl-3-methyl-2-butene	19.64	19.74	-0.10
2-Phenylethylamine	15.37	15.61	-0.24
2-Phenyloctane	25.20	25.25	-0.05
2-Phenylpropionitrile	15.77	15.99	-0.22
2-Phenyltetradecane	36.26	36.26	0.00
2-Phenyltetrahydropyran	19.48	19.59	-0.11
2-Phenyltoluene	22.30	22.23	0.07
2-Phenylvinyl bis(dipropylamino) phosphorus oxide	42.64	42.40	0.24
2-Phenylvinyl diethoxy phosphorus thioxide	29.94	29.68	0.26
2-Phenylvinyl dimethoxy phosphorus thioxide	26.05	25.98	0.07
2-Picoline	11.41	11.57	-0.16
2-Propanethiol	9.49	9.39	0.10
2-Propanol	7.03	6.92	0.11
2-Propene-1-thiol	9.08	9.27	-0.19
2-Propionylthiophene	15.75	15.59	0.16
2-Propoxy-4-methyl-1,3,2-dioxaphospholane	16.19	16.26	-0.07
2-Propoxyethanol	11.31	11.25	0.06
2-Propoxymethylthiophene	17.84	17.99	-0.15
2-Propoxyvinyl bis(dibutylamino) phosphorus oxide	45.89	46.03	-0.14
2-Propyl-1,4-diox-2-ene	13.90	13.84	0.06
2-Propyl-1,4-dioxane	14.17	14.19	-0.02
2-Propyl-2,3-dihydrofuran	13.18	13.29	-0.11
2-Propyl-2-hydroxy-1,4-dioxane	14.91	14.64	0.27
2-Propyl-3-ethyl-1,4-diox-2-ene	17.55	17.56	-0.01
2-Propyl-4-ethyl-2,3-dihydrofuran	16.82	16.99	-0.17
2-Propyl-4-ethylpyrrole	17.44	17.60	-0.16
2-Propyl-4-ethylpyrrolidine	17.75	17.81	-0.06
2-Propyl-4-isopropylpyrrolidine	19.50	19.63	-0.13
2-Propyl-4-methyl-2,3-dihydrofuran	15.04	15.15	-0.11
2-Propyl-4-methylpyrrole	15.70	15.76	-0.06
2-Propyl-4-methylpyrrolidine	15.97	15.97	0.00
2-Propyl-5-butylpyrrole	21.21	21.23	-0.02
2-Propyl-5-butylpyrrolidine	21.31	21.47	-0.16
2-Propyl-5-hexylpyrrole	24.89	24.90	-0.01
2-Propyl-5-hexylpyrrolidine	25.04	25.14	-0.10
2-Propyl-6-methyl-1,4-diox-2-ene	15.75	15.68	0.07
2-Propyl-6-methyl-2-hydroxy-1,4-dioxane	16.78	16.48	0.30

2-Propylcyclohexanone	16.23	16.61	-0.38
2-Propylheptanoic acid	19.77	19.82	-0.05
2-Propylnaphthalene	23.26	23.21	0.05
2-Propyloctanoic acid	21.61	21.66	-0.05
2-Propylpentanoic acid	16.17	16.15	0.02
2-Propylpiperidine	16.10	15.99	0.11
2-Propylpyridine	15.30	15.25	0.05
2-Propylpyrrole	14.31	13.90	0.41
2-Propyltetrahydropyran	15.34	15.36	-0.02
2-Propylthiophene	15.32	15.48	-0.16
2-Propyltoluene	17.98	18.00	-0.02
2-Propyn-1-butyrate	13.49	13.58	-0.09
2-Propyn-1-formate	8.02	8.13	-0.11
2-Propyn-1-heptanoate	19.02	19.09	-0.07
2-Propyn-1-hexanoate	17.18	17.25	-0.07
2-Propyn-1-ol	6.08	6.10	-0.02
2-Propyn-1-valerate	15.34	15.42	-0.08
2-Pyridinecarbonitrile	11.69	11.49	0.20
2-Pyridinecarboxaldehyde	11.90	11.78	0.12
2-Pyridinemethanamine	12.84	12.93	-0.09
2-Pyridinemethanol	12.07	12.13	-0.06
2-Pyridinepropanol	15.84	15.80	0.04
2-Pyrone	9.76	9.55	0.21
2-Pyrrolidone	8.57	8.69	-0.12
2-s-Butylphenol	18.46	18.61	-0.15
2-Silylpentasilane	29.00	28.97	0.03
2-Silyltetrasilane	24.23	24.20	0.03
2-Silyltrisilane	19.38	19.43	-0.05
2-t-Amylnaphthalene	26.92	26.87	0.05
2-t-Butyl-4-methylphenol	20.60	20.53	0.07
2-t-Butyl-6-methylphenol	20.43	20.53	-0.10
2-t-Butylaniline	19.43	19.53	-0.10
2-t-Butylfuran	14.85	14.91	-0.06
2-t-Butylnaphthalene	24.93	25.04	-0.11
2-t-Butylphenol	18.39	18.62	-0.23
2-t-Butyltetrahydropyran	17.14	17.18	-0.04
2-t-Butylthiophene	16.97	17.31	-0.34
2-t-Butyltoluene	19.68	19.82	-0.14
2-Tetralone	16.95	17.26	-0.31
2-Thiocresol	15.52	15.59	-0.07
2-Thiopheneacetonitrile	13.32	13.56	-0.24
2-Thiophenecarbaldehyde	12.25	12.02	0.23

2-Thiophenecarbonitrile	11.99	11.73	0.26
2-Thiophenemethanol	12.37	12.37	0.00
2-Tolunitrile	14.36	14.24	0.12
2-Tolyl 3-tolyl propoxyborine	32.55	32.45	0.10
2-Tolyl 4-tolyl propoxyborine	32.61	32.45	0.16
2-Tolyl dibutoxyborine	30.20	30.30	-0.10
2-Tolyl diethoxyborine	22.87	22.96	-0.09
2-Tolyl dimethoxyborine	19.08	19.26	-0.18
2-Tolyl dipropoxyborine	26.55	26.63	-0.08
2-Tridecanone	24.81	24.81	0.00
2-Trifluoromethylaniline	14.18	14.14	0.04
2-Undecanol	21.66	21.60	0.06
2-Undecanone	21.10	21.14	-0.04
2-Undecylthiacyclohexane	32.47	32.50	-0.03
2-Undecyne	20.29	20.44	-0.15
2-Vinyl-1,4-dioxane	12.07	12.23	-0.16
2-Vinylfuran	11.60	11.13	0.47
2-Vinyloxymethylthiophene	16.15	15.88	0.27
2-Vinylpyridine	13.29	13.29	0.00
2-Vinyltetrahydrofuran	11.48	11.56	-0.08
3-(1-Methyl-2-pyrrolidinyl)pyridine	19.62	19.50	0.12
3-(2-Furyl)-4-oxa-6-hexanol	17.92	17.99	-0.07
3-(2-Furyl)-4-oxa-6-hexyl acetate	22.86	23.05	-0.19
3-(4-Methyl-3-pentenyl)furan	18.44	18.52	-0.08
3-(Aminomethyl)-3,5,5-trimethylcyclohexanol	20.27	20.26	0.01
3-(Butylamino)propionitrile	15.03	14.95	0.08
3-(Chloromethyl)heptane	17.43	17.42	0.01
3-(Chloromethyl)pentane	13.64	13.75	-0.11
3-(Dibutylamino)propionitrile	22.44	22.47	-0.03
3-(Diethylamino)-1-propanol	16.06	15.77	0.29
3-(Diethylamino)propionitrile	15.09	15.13	-0.04
3-(Dimethylamino)butyronitrile	12.87	13.32	-0.45
3-(Dipentylamino)propionitrile	26.11	26.14	-0.03
3-(Dipropylamino)propionitrile	18.75	18.80	-0.05
3-(Ethylamino)propionitrile	11.38	11.28	0.10
3-(Hexylamino)propionitrile	18.75	18.62	0.13
3-(Methylamino)propionitrile	9.62	9.46	0.16
3-(Methylthio)-1-propene	11.15	11.12	0.03
3-(Pentylamino)propionitrile	16.88	16.78	0.10
3-(Propylamino)propionitrile	13.24	13.11	0.13
3-(Triethoxysilyl)-1-propanamine	23.48	23.48	0.00
3-(Trifluoromethyl)phenyl isocyanate	15.35	15.31	0.04

3-(Trimethylsilyl)-1-propanol	16.47	16.23	0.24
3,3,3-Trichloro-1-propene	12.03	12.07	-0.04
3,3,4,4-Tetrafluorodihydro-2,5-furandione	8.44	8.35	0.09
3,3,4,4-Tetramethyl-1,2-dioxetane	12.33	12.61	-0.28
3,3,4,4-Tetramethylhexane	18.96	19.19	-0.23
3,3,4-Trimethylhexane	17.28	17.34	-0.06
3,3,5-Trimethylcyclohexanone	16.60	16.60	0.00
3,3,5-Trimethylcyclohexyl acrylate	22.69	22.57	0.12
3,3,5-Trimethylheptane	19.02	19.18	-0.16
3,3'-Bitolyl	24.55	24.13	0.42
3,3-Diacetoxy-1-propene	14.72	14.90	-0.18
3,3-Diethoxy-1-propene	14.64	14.85	-0.21
3,3-Diethoxy-1-propyne	14.20	14.16	0.04
3,3'-Difluorobiphenyl	20.68	20.24	0.44
3,3-Dimethoxy-1-propene	11.27	11.15	0.12
3,3-Dimethyl-1-butanol	12.45	12.41	0.04
3,3-Dimethyl-1-butene	11.73	11.73	0.00
3,3-Dimethyl-1-pentene	13.48	13.56	-0.08
3,3-Dimethyl-2-butanol	12.48	12.42	0.06
3,3-Dimethyl-2-butylamine	12.97	13.18	-0.21
3,3-Dimethylbutanoic acid	12.49	12.49	0.00
3,3-Dimethylbutanoyl chloride	13.97	14.02	-0.05
3,3-Dimethylcyclohexanol	15.27	15.24	0.03
3,3-Dimethylcyclohexanone	14.74	14.78	-0.04
3,3-Dimethylheptane	17.31	17.36	-0.05
3,3-Dimethylhexane	15.46	15.52	-0.06
3,3-Dimethylhexanoic acid	16.10	16.16	-0.06
3,3-Dimethyloxetane	9.85	9.84	0.01
3,3-Dimethylpentane	13.60	13.69	-0.09
3,3-Dimethylpentanoic acid	14.27	14.32	-0.05
3,4,5-Trimethylheptane	19.10	19.15	-0.05
3,4-Dibromoheptane	19.85	19.87	-0.02
3,4-Dibromohexane	17.88	18.04	-0.16
3,4-Dichloro-1,4-dioxane	12.43	12.58	-0.15
3,4-Dichloro-1-butene	12.24	11.86	0.38
3,4-Dichlorotoluene	16.11	16.24	-0.13
3,4-Diethylhexane	19.06	19.17	-0.11
3,4-Dihydro-1H-2-benzopyran	15.75	15.98	-0.23
3,4-Dihydro-2H-1-benzopyran	15.67	16.00	-0.33
3,4-Dihydro-2H-1-benzopyran-2-one	16.16	16.02	0.14
3,4-Dihydro-2-methoxy-2H-pyran	11.90	12.04	-0.14
3,4-Dihydro-2-methyl-1(2H)-naphthalenone	19.24	19.07	0.17

3,4-Dihydro-4H-pyran	9.55	9.61	-0.06
3,4-Dihydroxytoluene	13.73	13.82	-0.09
3,4-Dimethoxybenzenemethanol	18.17	18.15	0.02
3,4-Dimethoxytoluene	17.61	17.59	0.02
3,4-Dimethyl-1-pentene	13.58	13.54	0.04
3,4-Dimethylacetophenone	18.31	18.17	0.14
3,4-Dimethylheptane	17.25	17.33	-0.08
3,4-Dimethylhexane	15.49	15.50	-0.01
3,4-Dimethyloctane	19.19	19.17	0.02
3,4-Dimethylthiophene	13.63	13.56	0.07
3,4-Hexanedione	11.99	12.07	-0.08
3,4-Lutidine	13.68	13.41	0.27
3,5,5-Trimethyl-1,1-hexanedithiol	23.48	23.40	0.08
3,5,5-Trimethyl-1-hexanol	17.94	17.90	0.04
3,5,5-Trimethyl-2-cyclohexenone	16.72	16.57	0.15
3,5-Bis(trifluoromethyl)aniline	15.89	16.16	-0.27
3,5-Diethyltoluene	19.85	19.90	-0.05
3,5-Dimethoxytoluene	17.60	17.59	0.01
3,5-Dimethyl-1-hexen-3-ol	15.80	15.93	-0.13
3,5-Dimethyl-2-cyclohexen-1-one	14.91	14.72	0.19
3,5-Dimethyl-4-heptanol	17.61	17.90	-0.29
3,5-Dimethylanisole	16.80	16.91	-0.11
3,5-Dimethylheptan-4-one	17.40	17.44	-0.04
3,5-Dimethylheptane	17.37	17.33	0.04
3,5-Dimethylisoxazole	10.29	10.29	0.00
3,5-Lupetidine	14.01	14.15	-0.14
3,5-Lutidine	13.40	13.41	-0.01
3,5-Xylidine	15.81	15.94	-0.13
3,6-Dibromononane	23.51	23.54	-0.03
3,6-Dihydro-4-methyl-2H-pyran	11.45	11.63	-0.18
3,6-Dimethyl-3-heptene	17.23	17.30	-0.07
3,6-Dimethyl-3-octanol	19.69	19.72	-0.03
3,6-Dimethyloctane	19.24	19.17	0.07
3,7,11-Trimethyl-2,6,10-dodecatrienal	28.75	28.43	0.32
3,7-Dimethyl-1,3,7-octatriene	19.39	18.98	0.41
3,7-Dimethyl-1,7-octanediol	20.19	20.28	-0.09
3,7-Dimethyl-1-octanol	19.80	19.73	0.07
3,7-Dimethyl-1-octene	19.07	19.05	0.02
3,7-Dimethyl-3-octanol	19.74	19.72	0.02
3-Acetyldihydro-2(3H)-furanone	11.71	11.80	-0.09
3-Allylpiperidine	15.61	15.88	-0.27
3-Amino-1,2-propanediol,	8.90	8.84	0.06

3-Aminobutyronitrile	9.17	9.47	-0.30
3-Aminopentane	11.34	11.36	-0.02
3-Aminopropionitrile	7.63	7.63	0.00
3-Anisaldehyde	15.44	15.21	0.23
3-Bromo-1,1,2-trichloro-1-propene	15.17	15.14	0.03
3-Bromo-1,1-dichloro-1-propene	13.45	13.19	0.26
3-Bromo-1-propanol	10.24	9.98	0.26
3-Bromo-2-methylnonane	22.10	22.27	-0.17
3-Bromo-3-methylpentane	14.93	14.99	-0.06
3-Bromo-4,5-dihydro-2(3H)-furanone	10.79	11.12	-0.33
3-Bromoaniline	15.29	15.13	0.16
3-Bromoanisole	16.34	16.11	0.23
3-Bromochlorobenzene	15.43	15.43	0.00
3-Bromocyclohexene	14.24	14.02	0.22
3-Bromofuran	10.31	10.47	-0.16
3-Bromohexane	14.83	14.95	-0.12
3-Bromonitrobenzene	16.03	16.17	-0.14
3-Bromononane	20.59	20.45	0.14
3-Bromopentane	13.10	13.11	-0.01
3-Bromopropanenitrile	9.34	9.34	0.00
3-Bromopropyne	8.67	8.61	0.06
3-Bromopyridine	12.48	12.61	-0.13
3-Bromothiophene	12.61	12.77	-0.16
3-Bromotoluene	15.34	15.43	-0.09
3-Buten-1-ol	8.63	8.63	0.00
3-Buten-2-one	7.94	8.17	-0.23
3-Butenoic acid	8.63	8.70	-0.07
3-Butoxypropanenitrile	14.30	14.28	0.02
3-Butyn-1-ol	7.92	7.94	-0.02
3-Butyn-2-ol	8.17	7.94	0.23
3-Butyn-2-one	7.56	7.49	0.07
3-Butynylbenzene	16.97	17.12	-0.15
3-Carene	17.59	17.41	0.18
3-Chloro-(1,1'-biphenyl)-2-ol	23.09	22.93	0.16
3-Chloro-1,1,1-trifluoropropane	8.20	8.37	-0.17
3-Chloro-1,1-diethoxypropane	17.04	16.87	0.17
3-Chloro-1-butanol	10.38	10.64	-0.26
3-Chloro-1-butene	10.01	9.95	0.06
3-Chloro-1-propanol	8.84	8.82	0.02
3-Chloro-2-(chloromethyl)-1-propene	11.85	11.90	-0.05
3-Chloro-2,5-furandione	10.01	9.92	0.09
3-Chloro-2-butanone	10.17	10.18	-0.01

3-Chloro-2-methylpropene	10.10	10.00	0.10
3-Chloro-3,4-epoxy-1-methylcyclohexane	14.75	14.73	0.02
3-Chloroacetophenone	16.08	16.27	-0.19
3-Chloroaniline	14.04	14.04	0.00
3-Chloroanisole	15.00	15.01	-0.01
3-Chlorobenzaldehyde	14.63	14.54	0.09
3-Chlorobenzeneacetonitrile	16.06	16.08	-0.02
3-Chlorobenzotrichloride	20.06	20.16	-0.10
3-Chlorobenzyl chloride	16.15	16.23	-0.08
3-Chlorobiphenyl	22.63	22.23	0.40
3-Chlorobutanoic acid	10.38	10.71	-0.33
3-Chlorocrotonic acid	11.12	10.65	0.47
3-Chlorocyclopentene	10.94	10.98	-0.04
3-Chloroheptane	15.63	15.58	0.05
3-Chlorohexane	13.83	13.75	0.08
3-Chloropentane	11.94	11.91	0.03
3-Chloropentanoic acid	12.57	12.55	0.02
3-Chlorophenol	13.17	13.12	0.05
3-Chloropropane-1,2-diyl dinitrate	14.19	14.30	-0.11
3-Chloropropanoyl chloride	10.26	10.42	-0.16
3-Chloropropionitrile	8.02	8.17	-0.15
3-Chloropropyl chloroformate	12.83	12.78	0.05
3-Chloropropyne	7.48	7.45	0.03
3-Chlorostyrene	16.16	16.04	0.12
3-Chlorotoluene	14.22	14.33	-0.11
3-Cyclohexene-1-carboxaldehyde	12.67	12.96	-0.29
3-Cyclohexene-1-carboxylic acid	13.16	13.39	-0.23
3-Cyclohexyl-1-propyne	17.48	17.53	-0.05
3-Cyclohexylhexane	21.68	21.99	-0.31
3-Decanol	19.76	19.76	0.00
3-Decanone	19.21	19.31	-0.10
3-Decen-2-one	19.32	19.23	0.09
3-Dimethylamino-1-propanol	12.26	12.13	0.13
3-Ethoxybenzaldehyde	17.37	17.06	0.31
3-Ethoxypropanenitrile	10.41	10.61	-0.20
3-Ethoxytoluene	17.10	16.85	0.25
3-Ethyl-1-pentene	13.59	13.56	0.03
3-Ethyl-2,4-dimethyl-1H-pyrrole	15.63	15.79	-0.16
3-Ethyl-2,4-pentanedione	14.07	13.89	0.18
3-Ethyl-2,5-dimethylpyrazine	16.48	16.45	0.03
3-Ethyl-2-methyl-1-pentene	15.31	15.42	-0.11
3-Ethyl-2-methylhexane	17.26	17.33	-0.07

3-Ethyl-2-methylpentane	15.40	15.50	-0.10
3-Ethyl-2-pentene	13.53	13.64	-0.11
3-Ethyl-3-methylhexane	17.24	17.36	-0.12
3-Ethyl-3-methylpentane	15.35	15.52	-0.17
3-Ethyl-4-methylhexane	17.10	17.33	-0.23
3-Ethyl-6-nonanone	20.89	21.13	-0.24
3-Ethyldecane	22.85	22.86	-0.01
3-Ethylheptane	17.41	17.35	0.06
3-Ethylhexane	15.44	15.52	-0.08
3-Ethyl-octane	19.22	19.19	0.03
3-Ethyl-o-xylene	17.97	18.07	-0.10
3-Ethylpentane	13.59	13.68	-0.09
3-Ethylpyridine	13.14	13.34	-0.20
3-Ethylstyrene	18.23	17.87	0.36
3-Ethyltoluene	16.12	16.16	-0.04
3-Fluoroaniline	12.02	12.09	-0.07
3-Fluoroanisole	13.04	13.06	-0.02
3-Fluorobenzaldehyde	12.80	12.59	0.21
3-Fluorobenzoyl chloride	14.85	14.54	0.31
3-Fluoronitrobenzene	12.96	13.12	-0.16
3-Fluorophenetole	14.85	14.90	-0.05
3-Fluorophenol	10.81	11.17	-0.36
3-Fluoropyridine	9.54	9.56	-0.02
3-Fluorotoluene	12.19	12.38	-0.19
3-Furancarboxaldehyde	10.00	9.60	0.40
3-Heptanol	14.17	14.26	-0.09
3-Heptanone	13.58	13.80	-0.22
3-Heptyne	13.12	13.10	0.02
3-Heptynoic acid	13.56	13.74	-0.18
3-Hexanol	12.44	12.42	0.02
3-Hexanone	11.87	11.97	-0.10
3-Hexanone ketazine	25.33	25.30	0.03
3-Hexanone O-ethyloxime	17.44	17.44	0.00
3-Hexanone O-propyloxime	19.26	19.27	-0.01
3-Hexanone oxime	13.55	13.57	-0.02
3-Hexyloxypropanenitrile	18.00	17.95	0.05
3-Hexyn-1-ol	11.71	11.82	-0.11
3-Hexyne	11.19	11.27	-0.08
3-Hexyne-2,5-diol	12.38	12.39	-0.01
3-Hydroxyacetophenone	15.28	15.06	0.22
3-Hydroxydiphenylether	21.82	21.72	0.10
3-Hydroxypropylphosphine	10.74	10.87	-0.13



3-Iodo-1-propanol	11.91	12.02	-0.11
3-Iodopentane	15.21	15.26	-0.05
3-Iodotoluene	17.47	17.40	0.07
3-Isopropyl-2-methyldecane	26.43	26.50	-0.07
3-Isopropyl-2-methyldodecane	30.12	30.17	-0.05
3-Isopropyl-2-methylheptane	20.91	20.99	-0.08
3-Isopropyl-2-methylnonane	24.60	24.66	-0.06
3-Isopropyl-2-methyloctane	22.76	22.82	-0.06
3-Isopropyl-2-methylundecane	28.26	28.33	-0.07
3-Isopropyltoluene	17.96	17.98	-0.02
3-Mercaptopropyl-trimethoxysilane	19.61	19.62	-0.01
3-Methoxy-1,2-propanediol	9.99	9.97	0.02
3-Methoxy-1-butanol	11.19	11.25	-0.06
3-Methoxyacetophenone	17.12	16.95	0.17
3-Methoxybenzenemethanol	15.55	15.56	-0.01
3-Methoxybenzonitrile	15.21	14.92	0.29
3-Methoxyphenol	13.88	13.80	0.08
3-Methoxyphenylacetone	18.39	18.78	-0.39
3-Methoxypropionitrile	8.80	8.76	0.04
3-Methoxypyridine	12.10	12.19	-0.09
3-Methoxytoluene	15.02	15.00	0.02
3-Methyl-1,2-butadiene	10.04	10.04	0.00
3-Methyl-1,3-pentadiene	12.03	11.69	0.34
3-Methyl-1,5-dibromopentane	17.88	17.98	-0.10
3-methyl-1,5-pentanediol	13.01	12.96	0.05
3-Methyl-1-butanethiol	13.07	13.05	0.02
3-Methyl-1-butene	9.98	9.89	0.09
3-Methyl-1-butyne	9.22	9.20	0.02
3-Methyl-1-heptanol	16.17	16.07	0.10
3-Methyl-1-hexene	13.63	13.56	0.07
3-Methyl-1-hexylamine	15.12	15.04	0.08
3-Methyl-1H-indene	17.22	17.10	0.12
3-Methyl-1H-pyrazole	9.25	9.11	0.14
3-Methyl-1-octyn-3-ol	17.24	17.10	0.14
3-Methyl-1-pentanol	12.21	12.40	-0.19
3-Methyl-1-pentene	11.69	11.72	-0.03
3-Methyl-1-pentyn-3-ol	11.59	11.59	0.00
3-Methyl-1-phenyl-1-butanone	19.95	19.85	0.10
3-Methyl-1-propylpyridinium bis(trifluoromethylsulfonyl)amide	30.28	30.30	-0.02
3-Methyl-2,5-furandione	9.96	9.83	0.13
3-Methyl-2-butanol	10.56	10.57	-0.01

3-Methyl-2-butanone	10.01	10.12	-0.11
3-Methyl-2-buten-1-ol	10.64	10.53	0.11
3-Methyl-2-butenal	10.33	10.18	0.15
3-Methyl-2-butenoyl chloride	12.47	12.14	0.33
3-Methyl-2-cyclohexen-1-one	13.13	12.90	0.23
3-Methyl-2-cyclopenten-1-one	10.98	11.07	-0.09
3-Methyl-2-heptanol	15.97	16.08	-0.11
3-Methyl-2-hexanol	14.18	14.24	-0.06
3-Methyl-2-oxazolidinone	9.28	9.49	-0.21
3-Methyl-2-oxobutanoic acid	10.82	10.75	0.07
3-Methyl-2-pentanol	12.29	12.41	-0.12
3-Methyl-2-pentanone	11.84	11.95	-0.11
3-Methyl-2-pentyl-2-cyclopenten-1-one	20.31	20.27	0.04
3-Methyl-3-buten-2-ol	10.31	10.49	-0.18
3-Methyl-3-heptanol	16.03	16.07	-0.04
3-Methyl-3-hexanol	14.25	14.23	0.02
3-Methyl-3-octanol	18.06	17.91	0.15
3-Methyl-3-pentanol	12.33	12.40	-0.07
3-Methyl-3-penten-1-yne	11.17	11.00	0.17
3-Methyl-4-heptanol	15.72	16.08	-0.36
3-Methyl-5-hepten-2-one	15.41	15.54	-0.13
3-Methyl-6-isopropyl-2-cyclohexen-1-ol	18.81	18.83	-0.02
3-Methyl-6-nonanone	19.35	19.29	0.06
3-Methylbenzaldehyde	14.69	14.53	0.16
3-Methylbenzenemethanamine	15.51	15.69	-0.18
3-Methylbenzoic acid	15.29	14.96	0.33
3-Methylbutanaloxime	11.75	11.80	-0.05
3-Methylbutanoic acid	10.62	10.64	-0.02
3-Methylbutanoyl chloride	12.16	12.17	-0.01
3-Methylbutyl 3-chloropropionate	18.14	18.11	0.03
3-Methylbutyl nitrate	13.19	13.03	0.16
3-Methylbutyl trichloroacetate	20.28	20.21	0.07
3-Methyl-cis-2-pentene	11.78	11.81	-0.03
3-Methylcyclohexanone	12.97	12.94	0.03
3-Methylcyclohexene	12.61	12.75	-0.14
3-Methylcyclohexyl acrylate	18.96	18.91	0.05
3-Methylcyclopentanol	11.64	11.56	0.08
3-Methylcyclopentanone	11.07	11.10	-0.03
3-Methylcyclopentene	10.92	10.92	0.00
3-Methyldecane	21.03	21.02	0.01
3-Methyldihydro-2,5-furandione	10.10	9.87	0.23
3-Methyldodecane	24.68	24.69	-0.01

3-Methyleicosane	39.39	39.37	0.02
3-Methyleneheptane	15.34	15.44	-0.10
3-Methylfuran	9.16	9.40	-0.24
3-Methylheneicosane	41.27	41.21	0.06
3-Methylheptadecane	33.91	33.87	0.04
3-Methylheptane	15.51	15.52	-0.01
3-Methylhexadecane	32.05	32.03	0.02
3-Methylhexanal	13.74	13.89	-0.15
3-Methylhexane	13.56	13.68	-0.12
3-Methylhexanoic acid	14.27	14.31	-0.04
3-Methylmethylenecyclohexane	14.74	14.57	0.17
3-Methylnonadecane	37.58	37.54	0.04
3-Methylnonane	19.10	19.19	-0.09
3-Methyloctadecane	35.75	35.70	0.05
3-Methyloctane	17.34	17.35	-0.01
3-Methylpentadecane	30.23	30.20	0.03
3-Methylpentadecane-3-ol	30.77	30.75	0.02
3-Methylpentane	11.81	11.84	-0.03
3-Methylpiperidine	12.44	12.33	0.11
3-Methylpyridazine	10.76	10.75	0.01
3-Methylpyridine	11.43	11.51	-0.08
3-Methylquinoline	18.61	18.47	0.14
3-Methylstyrene	16.22	16.04	0.18
3-Methylsulfolane	12.66	12.63	0.03
3-Methyltetradecane	28.40	28.36	0.04
3-Methylthiophene	11.58	11.70	-0.12
3-Methyl-trans-2-pentene	11.78	11.81	-0.03
3-Methyltridecane	26.47	26.53	-0.06
3-Methylundecane	22.87	22.86	0.01
3-Methylvaleric acid	12.47	12.48	-0.01
3-Nitro-2-butanol	11.08	10.92	0.16
3-Nitrobenzotrifluoride	14.77	15.17	-0.40
3-Nitrobenzylalcohol	15.51	15.62	-0.11
3-Nitrotoluene	14.88	15.06	-0.18
3-Nonanol	17.87	17.93	-0.06
3-Nonanone	17.34	17.47	-0.13
3-Nonenoic acid	17.83	17.92	-0.09
3-Octanol	16.00	16.09	-0.09
3-Octanone	15.48	15.64	-0.16
3-Octyne	14.84	14.94	-0.10
3-Oxa-5-oxo-1-octanol	14.98	15.03	-0.05
3-Pentanethiol	13.07	13.06	0.01

3-Pentanol	10.56	10.59	-0.03
3-Pentanone ketazine	21.59	21.63	-0.04
3-Pentanone O-ethyloxime	15.55	15.60	-0.05
3-Pentanone O-propyloxime	17.36	17.44	-0.08
3-Pentanone oxime	11.73	11.73	0.00
3-Penten-2-ol	10.55	10.51	0.04
3-Pentyloxypropanenitrile	16.15	16.12	0.03
3-Pentyn-1-ol	9.87	9.99	-0.12
3-Phenoxybenzaldehyde	23.29	23.13	0.16
3-Phenyl-2-propyn-1-ol	16.34	16.05	0.29
3-Phenylpropene	15.79	15.97	-0.18
3-Phenylpropylthiol	19.02	19.13	-0.11
3-Phenyltoluene	22.32	22.23	0.09
3-Piperidinemethanol	13.01	12.89	0.12
3-Propoxy-1-propene	12.17	12.41	-0.24
3-Propoxypropanenitrile	12.47	12.45	0.02
3-Propyltoluene	18.06	18.00	0.06
3-Pyridinemethanamine	12.88	12.87	0.01
3-Pyridinemethanol	12.10	12.07	0.03
3-Pyridinepropanol	15.84	15.74	0.10
3-t-Butylfuran	14.70	14.90	-0.20
3-t-Butylthiophene	17.12	17.20	-0.08
3-t-Butyltoluene	19.78	19.82	-0.04
3-Thiocresol	15.52	15.59	-0.07
3-Thiopropionic acid	10.06	10.03	0.03
3-Tolunitrile	13.80	14.24	-0.44
3-Tolyl dibutoxyborine	30.32	30.30	0.02
3-Tolyl diethoxyborine	23.02	22.96	0.06
3-Tolyl dimethoxyborine	19.18	19.26	-0.08
3-Tolyl dipropoxyborine	26.66	26.63	0.03
3-Tolylphosphorous diaziridide	25.24	25.25	-0.01
3-Trifluoromethylaniline	13.87	14.14	-0.27
3-Trifluoromethylbenzonitrile	14.25	14.35	-0.10
3-Trifluoromethylbenzoyl chloride	16.89	16.60	0.29
3-Vinyl-7-oxabicyclo[4.1.0]heptane	14.33	14.37	-0.04
3-Vinylpyridine	13.50	13.22	0.28
4-(1,1-Dimethylpropyl)cyclohexanone	20.15	20.27	-0.12
4(10)-Thujene-3-ol	18.30	17.93	0.37
4-(1-Butylpentyl)pyridine	26.26	26.17	0.09
4-(1-Ethylpropyl)pyridine	18.84	18.83	0.01
4-(1-Methylvinyl)-1-cyclohexene-1-methanol	16.64	16.89	-0.25
4-(2-Furanyl)-2-butanone	14.74	15.03	-0.29

4-(3-Cyclohexen-1-yl)pyridine	19.57	19.74	-0.17
4-(3-Phenylpropyl)pyridine	24.75	24.91	-0.16
4-(Ethylthio)-toluene	19.38	19.46	-0.08
4-(Methylthio)aniline	17.46	17.24	0.22
4-(Pentyloxy)benzoyl chloride	24.45	24.52	-0.07
4,4'-Diisocyanatodiphenylmethane	27.99	27.72	0.27
4,4-Dimethyl-1-pentene	13.26	13.56	-0.30
4,4-Dimethyl-1-pentyne	12.89	12.88	0.01
4,4-Dimethyl-2-pentanone	13.67	13.79	-0.12
4,4-Dimethyl-2-pentyne	13.08	13.09	-0.01
4,4-Dimethylcyclohexanone	14.53	14.78	-0.25
4,4-Dimethylheptane	17.35	17.36	-0.01
4,5-Dichloro-1,3-dioxolan-2-one	10.78	10.68	0.10
4,5-Diethyloctane	22.76	22.84	-0.08
4,5-Dihydro-2-methylthiazole	11.42	11.55	-0.13
4-Acetylmorpholine	13.11	13.17	-0.06
4-Acetylpyridine	13.48	13.45	0.03
4-Allyl anisole	18.49	18.55	-0.06
4-Allyl-2-methoxyphenol	19.19	19.25	-0.06
4-Allyl-2-methoxyphenyl acetate	23.02	23.00	0.02
4-Allylphenol	16.46	16.67	-0.21
4-Amino-1-butanol	10.06	10.11	-0.05
4-Benzylpiperidine	21.65	22.07	-0.42
4-Benzylpyridine	21.09	21.24	-0.15
4-Bromo-1,2-butadiene	11.33	11.24	0.09
4-Bromo-1,2-dimethoxybenzene	18.91	18.69	0.22
4-Bromo-1-butene	11.13	11.13	0.00
4-Bromo-2-methylhexane	16.78	16.77	0.01
4-Bromoacetophenone	17.41	17.37	0.04
4-Bromoanisole	16.56	16.11	0.45
4-Bromobutyronitrile	11.17	11.17	0.00
4-Bromocrotonic acid ethylester	15.85	15.54	0.31
4-Bromodiphenyl ether	24.20	24.03	0.17
4-Bromophenyltrimethylsilane	22.67	22.91	-0.24
4-Bromopyridine	12.48	12.61	-0.13
4-Bromotetradecane	29.28	29.63	-0.35
4-Bromotoluene	15.42	15.43	-0.01
4-Bromotridecane	27.51	27.80	-0.29
4-Butylacetophenone	22.09	21.77	0.32
4-Butylmorpholine	16.67	16.87	-0.20
4-Butylphenol	18.44	18.63	-0.19
4-Chloro-1-(4-fluorophenyl)-1-butanone	19.99	19.90	0.09

4-Chloro-1,2-butadiene	10.04	10.08	-0.04
4-Chloro-1-butanol	10.66	10.65	0.01
4-Chloro-1-butene	9.93	9.97	-0.04
4-Chloro-1-phenyl-1-butanone	20.16	19.93	0.23
4-Chloro-1-trifluoromethoxybenzene	14.89	14.84	0.05
4-Chloro-2-pentene	11.97	11.83	0.14
4-Chloroacetophenone	16.50	16.27	0.23
4-Chloroaniline	13.88	14.04	-0.16
4-Chloroanisole	14.74	15.01	-0.27
4-Chlorobenzaldehyde	14.96	14.54	0.42
4-Chlorobenzenemethanethiol	17.64	17.37	0.27
4-Chlorobutanal	10.20	10.30	-0.10
4-Chlorobutanoic acid	10.96	10.73	0.23
4-Chlorobutanoyl chloride	12.21	12.26	-0.05
4-Chlorobutyronitrile	9.92	10.01	-0.09
4-Chlorodiphenyl ether	23.05	22.93	0.12
4-Chloroethylbenzene	16.14	16.17	-0.03
4-Chloroheptane	15.63	15.58	0.05
4-Chloronitrobenzene	15.04	15.07	-0.03
4-Chloro-N-methylaniline	16.06	15.98	0.08
4-Chloropentanoic acid	12.53	12.55	-0.02
4-Chlorophenol	12.99	13.12	-0.13
4-Chlorophenoxytriethylsilane	27.61	27.50	0.11
4-Chlorostyrene	16.49	16.04	0.45
4-Chlorothiophenol	15.29	15.59	-0.30
4-Chlorotoluene	14.14	14.33	-0.19
4-Cumylphenol	16.65	16.78	-0.13
4-Decanol	19.70	19.76	-0.06
4-Decanone	19.18	19.31	-0.13
4-Diethylamino-2-butanol	17.44	17.61	-0.17
4-Ethoxyacetanilide	20.53	20.43	0.10
4-Ethoxyaniline	16.33	16.56	-0.23
4-Ethoxytoluene	16.86	16.85	0.01
4-Ethyl-2-methylhexane	17.37	17.33	0.04
4-Ethyl-2-propylthiophane	19.77	19.64	0.13
4-Ethyl-2-propylthiophane sulfone	19.88	19.97	-0.09
4-Ethyl-3-oxa-1-heptanol	16.64	16.76	-0.12
4-Ethyl-3-oxa-5-oxo-1-octanol	18.64	18.71	-0.07
4-Ethyl-4-heptanol	17.81	17.91	-0.10
4-Ethylaniline	15.94	15.87	0.07
4-Ethylheptane	17.38	17.35	0.03
4-Ethyl-m-xylene	17.97	18.07	-0.10

4-Ethylnitrobenzene	16.94	16.90	0.04
4-Ethyl-octane	19.24	19.19	0.05
4-Ethyl-o-xylene	18.07	18.07	0.00
4-Ethylphenyldiallylphosphine	29.26	29.06	0.20
4-Ethylphenyldipropylphosphine	29.55	29.30	0.25
4-Ethylpyridine	13.29	13.34	-0.05
4-Ethylstyrene	18.22	17.87	0.35
4-Ethyltoluene	16.15	16.16	-0.01
4-Fluoro-1-trichloromethoxybenzene	18.77	18.82	-0.05
4-Fluoro-1-trifluoromethoxybenzene	12.88	12.89	-0.01
4-Fluoro-2-methylaniline	13.74	13.99	-0.25
4-Fluoroacetophenone	14.35	14.32	0.03
4-Fluoroanisole	12.95	13.06	-0.11
4-Fluorobenzeneacetonitrile	13.84	14.13	-0.29
4-Fluorobenzonitrile	12.59	12.30	0.29
4-Fluorobenzoyl chloride	14.46	14.54	-0.08
4-Fluoriodobenzene	15.28	15.46	-0.18
4-Fluoronitrobenzene	13.02	13.12	-0.10
4-Fluorophenetole	14.80	14.90	-0.10
4-Fluorophenyltrimethylsilane	19.95	19.86	0.09
4-Fluorotoluene	12.21	12.38	-0.17
4-Formylmorpholine	11.34	11.39	-0.05
4-Heptanamine	14.98	15.03	-0.05
4-Heptanol	14.26	14.26	0.00
4-Heptanone	13.63	13.80	-0.17
4-Heptanone ketazine	29.07	28.97	0.10
4-Heptanone O-ethyloxime	19.28	19.27	0.01
4-Heptanone O-propyloxime	21.13	21.11	0.02
4-Heptanone oxime	15.38	15.40	-0.02
4-Heptyl bromide	16.79	16.78	0.01
4-Hexen-2-ol	12.43	12.34	0.09
4-Hexen-3-one	11.95	11.89	0.06
4-Hexylacetophenone	25.71	25.44	0.27
4H-Pyran-4-one	9.79	9.48	0.31
4-Hydroxy-2-butanone	9.32	8.86	0.46
4-Hydroxy-4-methyl-2-pentanone	12.45	12.51	-0.06
4-Iodo-1,2-butadiene	13.68	13.28	0.40
4-Iodotoluene	17.10	17.40	-0.30
4-Isopropyl-2-propylthiophane	21.52	21.46	0.06
4-Isopropyl-2-propylthiophane sulfone	21.65	21.79	-0.14
4-Isopropylbenzaldehyde	18.61	18.19	0.42
4-Isopropylcyclohexanone	16.58	16.59	-0.01

4-Isopropylheptane	19.22	19.17	0.05
4-Isopropylphenyldiallylphosphine	31.03	30.88	0.15
4-Isopropylpyridine	14.96	15.16	-0.20
4-Isopropylstyrene	20.03	19.69	0.34
4-Methoxy-2-methylaniline	16.63	16.62	0.01
4-Methoxy-4-methyl-2-pentanone	14.48	14.44	0.04
4-Methoxy- $\alpha$ -methylbenzenemethanol	17.29	17.40	-0.11
4-Methoxyaniline	14.65	14.71	-0.06
4-Methoxybenzeneacetaldehyde	16.93	17.05	-0.12
4-Methoxybenzeneacetonitrile	16.64	16.76	-0.12
4-Methoxybenzenemethanamine	16.40	16.36	0.04
4-Methoxybenzenethiol	17.99	18.04	-0.05
4-Methoxyphenyldiallylphosphine	28.13	27.90	0.23
4-Methoxyphenyldibutylphosphine	32.05	31.82	0.23
4-Methoxyphenyldipentylphosphine	35.89	35.49	0.40
4-Methoxytoluene	14.98	15.00	-0.02
4-Methyl-1,3-dioxane	10.41	10.43	-0.02
4-Methyl-1,3-dioxolane	8.51	8.60	-0.09
4-Methyl-1-heptanol	16.38	16.07	0.31
4-Methyl-1-hexene	13.59	13.56	0.03
4-Methyl-1H-imidazole	9.25	9.22	0.03
4-Methyl-1-pentene	11.71	11.72	-0.01
4-Methyl-1-pentyne	11.12	11.04	0.08
4-Methyl-2-(1-hexen-5-yl)phenol	23.97	24.08	-0.11
4-Methyl-2,6-di(3-hexen-2-yl)phenol	35.03	35.10	-0.07
4-Methyl-2,6-dicrotylphenol	27.58	27.79	-0.21
4-Methyl-2-crotylphenol	20.12	20.45	-0.33
4-Methyl-2-heptanol	16.41	16.08	0.33
4-Methyl-2-hexanamine	14.94	15.01	-0.07
4-Methyl-2-nitrophenol	16.17	15.76	0.41
4-Methyl-2-pentanol	12.43	12.41	0.02
4-Methyl-2-pentenoic acid	12.73	12.40	0.33
4-Methyl-2-pentyne	11.24	11.25	-0.01
4-Methyl-3-heptanol	16.13	16.08	0.05
4-Methyl-3-penten-2-ol	12.40	12.37	0.03
4-Methyl-4-heptanol	16.03	16.07	-0.04
4-Methylacetophenone	16.43	16.27	0.16
4-Methylbenzaldehyde	14.78	14.53	0.25
4-Methylbenzeneacetaldehyde	16.23	16.37	-0.14
4-Methylbenzeneacetonitrile	15.91	16.08	-0.17
4-Methylbenzenemethanamine	15.69	15.69	0.00
4-Methylbenzenepropanal	18.02	18.20	-0.18



4-Methylbenzoyl chloride	16.82	16.49	0.33
4-Methyl-cis-2-pentene	11.55	11.77	-0.22
4-Methylcyclohexanemethanol	15.39	15.21	0.18
4-Methylcyclohexanone	12.95	12.94	0.01
4-Methylcyclohexene	12.61	12.75	-0.14
4-Methylcyclohexyl acrylate	18.97	18.91	0.06
4-Methylcyclopentene	10.81	10.92	-0.11
4-Methyldecane	21.01	21.02	-0.01
4-Methyldocosane	43.08	43.05	0.03
4-Methyldodecane	24.68	24.69	-0.01
4-Methyleicosane	39.41	39.37	0.04
4-Methylene-1-isopropylcyclohexene	18.16	18.19	-0.03
4-Methylene-2-oxetanone	8.04	7.79	0.25
4-Methylheneicosane	41.22	41.21	0.01
4-Methylheptadecane	33.91	33.87	0.04
4-Methylheptane	15.51	15.52	-0.01
4-Methylhexadecane	32.06	32.03	0.03
4-Methylnonadecane	37.57	37.54	0.03
4-Methylnonane	19.18	19.19	-0.01
4-Methyloctadecane	35.71	35.70	0.01
4-Methyloctane	17.36	17.35	0.01
4-Methyloxazole	8.41	8.37	0.04
4-Methylpent-3-en-2-one	11.94	11.92	0.02
4-Methylpentadecane	30.21	30.20	0.01
4-Methylpentyl 4-methylpentoxy dithiophosphinic acid	33.08	33.17	-0.09
4-Methylpentyl dichloro phosphorus oxide	18.92	19.07	-0.15
4-Methylpentyl dichloro phosphorus thioxide	22.42	22.37	0.05
4-Methylpentyl isopropoxy dithiophosphinic acid	27.75	27.68	0.07
4-Methylpentyl octyloxy dithiophosphinic acid	36.56	36.86	-0.30
4-Methylphenethyl alcohol	16.54	16.72	-0.18
4-Methylpiperidine	12.08	12.33	-0.25
4-Methylpyridine	11.44	11.51	-0.07
4-Methylpyrimidine	10.66	10.41	0.25
4-Methylquinoline	18.41	18.47	-0.06
4-Methylstyrene	16.07	16.04	0.03
4-Methyltetradecane	28.33	28.36	-0.03
4-Methyl-trans-2-pentene	11.80	11.77	0.03
4-Methyltridecane	26.46	26.53	-0.07
4-Methylundecane	22.89	22.86	0.03
4-Methylvaleronitrile	11.78	11.76	0.02
4-Morpholinamine	10.81	10.89	-0.08

4-Morpholineethanamine	14.59	14.56	0.03
4-Morpholineethanol	13.70	13.76	-0.06
4-Morpholinepropanamine	16.37	16.39	-0.02
4-Nitroanisole	15.70	15.74	-0.04
4-Nitromethyltoluene	16.42	16.60	-0.18
4-Nonanol	17.85	17.93	-0.08
4-Nonanone	17.38	17.47	-0.09
4-Nonylphenol	27.64	27.80	-0.16
4-Octanol	16.12	16.09	0.03
4-Octanone	15.70	15.64	0.06
4-Octylacetophenone	29.47	29.12	0.35
4-Octyne	14.87	14.94	-0.07
4-Oxa-6-oxo-2-nonanol	16.77	16.87	-0.10
4-Oxo-1-heptanol	14.19	14.36	-0.17
4-Oxopentanal	10.03	10.34	-0.31
4-Oxopentanoic acid	10.69	10.77	-0.08
4-Penten-1-ol	10.45	10.46	-0.01
4-Penten-2-ol	10.38	10.46	-0.08
4-Pentenal	9.89	10.11	-0.22
4-Pentenitrile	9.90	9.82	0.08
4-Pentenoic acid	10.41	10.54	-0.13
4-Pentylphenol	20.86	20.46	0.40
4-Pentyn-1-ol	9.65	9.78	-0.13
4-Phenoxyphenyldiallylphosphine	35.49	35.82	-0.33
4-Phenyl-1,3-dioxane	18.23	18.33	-0.10
4-Phenyl-2-butanone	17.87	18.03	-0.16
4-Piperidineethanol	14.74	14.73	0.01
4-Propyldecane	24.74	24.69	0.05
4-Propyldocosane	46.71	46.72	-0.01
4-Propyldodecane	28.37	28.36	0.01
4-Propylheneicosane	44.92	44.88	0.04
4-Propylheptane	19.23	19.19	0.04
4-Propylnonane	22.85	22.86	-0.01
4-Propyloctane	21.02	21.02	0.00
4-Propylphenol	16.73	16.79	-0.06
4-Propylpyridine	14.97	15.18	-0.21
4-Propyltoluene	18.07	18.00	0.07
4-Propyltridecane	30.21	30.20	0.01
4-Propylundecane	26.55	26.53	0.02
4-Pyridineethanamine	14.71	14.70	0.01
4-Pyridinemethanamine	12.73	12.87	-0.14
4-s-Butylaniline	19.44	19.52	-0.08

4-s-Butylphenol	18.31	18.61	-0.30
4-t-Butyl-2-methylphenol	20.61	20.53	0.08
4-t-Butylacetophenone	21.97	21.77	0.20
4-t-Butylaniline	19.43	19.53	-0.10
4-t-Butylbenzaldehyde	20.38	20.03	0.35
4-t-Butylphenol	18.59	18.62	-0.03
4-t-Butylpyridine	17.10	17.01	0.09
4-tert-Butyltoluene	19.79	19.82	-0.03
4-Tetradecanol	27.19	27.11	0.08
4-Tolyl dibutoxyborine	30.39	30.30	0.09
4-Tolyl diethoxyborine	23.01	22.96	0.05
4-Tolyl dimethoxyborine	19.22	19.26	-0.04
4-Tolyl dipropoxyborine	26.73	26.63	0.10
4-Tolylacetate	17.11	16.87	0.24
4-Tolyldiallylphosphine	26.91	27.22	-0.31
4-Tolyliodoacetylene	20.19	20.41	-0.22
4-Tolylphosphorous diaziridide	25.36	25.25	0.11
4-Tridecanol	25.32	25.27	0.05
4-Trifluoromethylaniline	14.18	14.14	0.04
4-Trifluoromethylphenyltrimethylsilane	21.66	21.92	-0.26
4-Trimethylsiloxyphenyltrimethylsilane	29.58	29.55	0.03
4-Vinylcyclohexene	14.25	14.46	-0.21
4-Vinylpyridine	13.33	13.22	0.11
5-(Chloromethyl)-1,3-benzodioxole	16.82	16.74	0.08
5,5-Dimethyl-1-hexen-3-yne	14.77	14.81	-0.04
5,5-Dimethyl-1-hexene	15.46	15.40	0.06
5,6,7,8-Tetrahydro-1-naphthalenamine	18.54	18.76	-0.22
5,6,7,8-Tetrahydroquinoline	16.17	16.30	-0.13
5,6-Dibutyldecane	33.75	33.85	-0.10
5-Amino-1-pentanol	11.84	11.94	-0.10
5-Amino-2-butoxypyridine	19.85	19.54	0.31
5-Aminomethyl-1,3-benzodioxole	16.04	16.20	-0.16
5-Bromo-1-pentene	12.96	12.97	-0.01
5-Bromo-3-bromomethyl-2-methyloetane	25.56	25.33	0.23
5-Bromo-3-bromomethyloctane	23.42	23.51	-0.09
5-Bromoacenaphthene	23.61	23.61	0.00
5-Bromononane	20.58	20.45	0.13
5-Bromovaleronitrile	13.00	13.01	-0.01
5-Butyldocosane	48.51	48.55	-0.04
5-Butylnonane	24.59	24.69	-0.10
5-Chloro-2-pentanone	11.91	12.03	-0.12
5-Chloroacenaphthene	22.23	22.51	-0.28

5-Chloropentanoyl chloride	14.01	14.09	-0.08
5-Chlorovaleric acid	12.53	12.56	-0.03
5-Cyclohexyleicosane	47.71	47.69	0.02
5-Decanol	19.80	19.76	0.04
5-Decyn-1-ol	18.99	19.17	-0.18
5-Decyne	18.52	18.61	-0.09
5-Ethyl-2-norbornene	15.52	15.54	-0.02
5-Ethylidene-2-norbornene	15.42	15.51	-0.09
5-Ethyl-m-xylene	18.12	18.07	0.05
5-Hexenoic acid	12.27	12.37	-0.10
5-Hexyn-2-one	11.00	11.16	-0.16
5-Hydroxy-2-pentanone	10.58	10.69	-0.11
5-Iodoacenaphthene	25.38	25.58	-0.20
5-Isopropyl-2-methylphenol	18.61	18.68	-0.07
5-Methoxy-1-cyclohexyl-1-pentanol	23.20	23.23	-0.03
5-Methoxy-1-phenyl-1-pentanol	22.71	22.82	-0.11
5-Methoxy-2-pentanol	13.16	13.08	0.08
5-Methoxy-2-pentanone	12.47	12.63	-0.16
5-Methyl-1-heptanol	16.26	16.07	0.19
5-Methyl-1-hexanol	14.16	14.24	-0.08
5-Methyl-1-hexene	13.62	13.56	0.06
5-Methyl-1-hexyne	12.87	12.87	0.00
5-Methyl-2(3H)-furanone	9.60	9.67	-0.07
5-Methyl-2(5H)-furanone	9.58	9.80	-0.22
5-Methyl-2,3-hexanedione	13.92	13.89	0.03
5-Methyl-2-ethylcoumaran	19.77	19.75	0.02
5-Methyl-2-furanmethanol	11.84	11.85	-0.01
5-Methyl-2-hexanol	14.26	14.24	0.02
5-Methyl-2-hexanone oxime	15.34	15.39	-0.05
5-Methyl-2-hexyne	13.01	13.09	-0.08
5-Methyl-2-isopropylcyclohexanol acetate	22.72	22.67	0.05
5-Methyl-3-heptanol	15.92	16.08	-0.16
5-Methyl-3-hexanol	14.05	14.24	-0.19
5-Methyl-3-hexen-2-one	13.70	13.71	-0.01
5-Methyl-5-hexen-2-one	13.71	13.71	0.00
5-Methylbenzo[b]thiophene	18.46	18.25	0.21
5-Methyldecane	21.03	21.02	0.01
5-Methyldocosane	43.10	43.05	0.05
5-Methyldodecane	24.64	24.69	-0.05
5-Methyleicosane	39.42	39.37	0.05
5-Methylheneicosane	41.24	41.21	0.03
5-Methylheptadecane	33.90	33.87	0.03

5-Methylhexadecane	32.08	32.03	0.05
5-Methylisoxazole	8.46	8.54	-0.08
5-Methylnonadecane	37.57	37.54	0.03
5-Methylnonane	19.14	19.19	-0.05
5-Methyloctadecane	35.73	35.70	0.03
5-Methylpentadecane	30.21	30.20	0.01
5-Methylquinoline	18.45	18.47	-0.02
5-Methyltetradecane	28.33	28.36	-0.03
5-Methyltetralin	18.83	19.05	-0.22
5-Methyltricosane	44.94	44.88	0.06
5-Methyltridecane	26.54	26.53	0.01
5-Methylundecane	22.83	22.86	-0.03
5-Methyluracil	11.23	11.56	-0.33
5-Nonanol	17.93	17.93	0.00
5-Nonanone	17.35	17.47	-0.12
5-Oxohexanoic acid	12.60	12.60	0.00
5-Phenyl-1-pentanol	20.21	20.32	-0.11
5-Phenyl-4-nonene	26.61	27.05	-0.44
5-Phenyleicosane	47.55	47.27	0.28
5-Phenylnonane	27.12	27.09	0.03
5-Propyl-4-tridecanol	30.60	30.76	-0.16
6,6-Dimethylbicyclo(3.1.1)heptan-2-one	15.83	15.74	0.09
6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-ethanol	19.69	19.81	-0.12
6,7-Diamyldodecane	41.25	41.19	0.06
6-Bromo-2-hexanone	14.91	15.04	-0.13
6-Bromoundecane	24.32	24.12	0.20
6-Chloro-1-hexanol	14.35	14.32	0.03
6-Dodecyne	22.32	22.28	0.04
6-Heptenoic acid	14.08	14.21	-0.13
6-Methyl-1-heptanol	16.15	16.07	0.08
6-Methyl-1-heptene	15.47	15.39	0.08
6-Methyl-2-heptanol	16.02	16.08	-0.06
6-Methyl-2-heptanol acetate	20.09	19.88	0.21
6-Methyl-2-heptanone	15.65	15.62	0.03
6-Methyl-3-heptanol	16.07	16.08	-0.01
6-Methyl-4-octanone	17.37	17.46	-0.09
6-Methyldodecane	24.73	24.69	0.04
6-Methylpentadecane	30.15	30.20	-0.05
6-Methylquinoline	18.61	18.47	0.14
6-Methyltetradecane	28.37	28.36	0.01
6-Methyltridecane	26.52	26.53	-0.01
6-Methylundecane	22.88	22.86	0.02

6-Oxabicyclo[3.1.0]hexane	9.00	9.01	-0.01
6-Undecanol	21.36	21.60	-0.24
6-Undecanone	20.86	21.14	-0.28
6-Vinyl-6-methyl-1-isopropyl-3-(1-methylethylidene)cyclohexene	27.72	27.31	0.41
7-(3-Phenylpropyl)-7-tridecanol	40.73	40.49	0.24
7,8-Dimethyltetradecane	30.04	30.18	-0.14
7-Bromo-1,5,5-trichloroheptane	22.42	22.48	-0.06
7-Butyl-7-tridecanol	32.65	32.59	0.06
7-Butyltridecane	31.95	32.03	-0.08
7-Chloro-1-heptanol	16.17	16.16	0.01
7-Chloroheptanonitrile	15.50	15.52	-0.02
7-Hexyl-7-pentadecanol	39.69	39.93	-0.24
7-Hexylpentadecane	39.26	39.37	-0.11
7-Methylpentadecane	30.19	30.20	-0.01
7-Methylquinoline	18.67	18.47	0.20
7-Methyltetradecane	28.35	28.36	-0.01
7-Methyltridecane	26.55	26.53	0.02
7-Oxabicyclo[4.1.0]heptane	10.86	10.84	0.02
7-Phenyl-6-tridecene	34.23	34.39	-0.16
7-Phenyltridecane	34.40	34.43	-0.03
8-Chloroquinoline	18.22	18.48	-0.26
8-Heptyl-7-pentadecene	41.27	41.17	0.10
8-Heptylpentadecane	41.29	41.21	0.08
8-Methylpentadecane	30.19	30.20	-0.01
8-Methylquinoline	18.51	18.47	0.04
8-Propyl-8-pentadecanol	34.51	34.42	0.09
8-Propylpentadecane	33.90	33.87	0.03
9,10,11,12-Tetrapropyleicosane	59.23	59.52	-0.29
9,10-Benzophenanthrene	32.24	31.87	0.37
9,10-Dimethyloctadecane	37.09	37.52	-0.43
9,10-Dipropyloctadecane	44.76	44.86	-0.10
9-Bromo-1,5,5-trichlorononane	26.20	26.15	0.05
9-Decen-1-ol	19.63	19.64	-0.01
9-Decyn-1-ol	18.99	18.95	0.04
9-Heptylheptadecane	44.74	44.88	-0.14
9-methyl-8-heptadecene	33.79	33.83	-0.04
Acenaphthene	20.55	20.60	-0.05
Acetaldehyde	4.57	4.73	-0.16
Acetaldoxime	6.22	6.31	-0.09
Acetamide	6.03	5.77	0.26
Acetic acid	5.17	5.15	0.02

Acetic acid 1,3-dichloroisopropylester	14.34	14.53	-0.19
Acetic acid 1-chloroethylester	10.82	10.83	-0.01
Acetic acid 2-bromoethylester	11.91	11.95	-0.04
Acetic acid 2-chloroethylester	10.51	10.79	-0.28
Acetic acid 2-phenoxyethylester	19.21	19.31	-0.10
Acetic acid 3-chloropropylester	12.88	12.62	0.26
Acetic anhydride	8.87	8.90	-0.03
Acetoacetic acid butylester	16.19	16.33	-0.14
Acetoin	8.74	8.86	-0.12
Acetol	7.01	7.02	-0.01
Acetone dibutoxyketal	22.29	22.27	0.02
Acetone glycerol	12.93	12.81	0.12
Acetone oxime	7.97	8.06	-0.09
Acetonitrile	4.39	4.44	-0.05
Acetonylacetone	11.84	12.07	-0.23
Acetophenone	14.47	14.36	0.11
Acetoxime O-ethyl ether	10.28	10.18	0.10
Acetoxime O-methyl ether	8.41	8.33	0.08
Acetoxime O-propyl ether	12.06	12.01	0.05
Acetoxyacetic acid ethylester	13.23	13.25	-0.02
Acetoxyacetone	10.69	10.83	-0.14
Acetylacetone (enol form)	10.96	10.55	0.41
Acetylbromide	7.86	7.85	0.01
Acetylchloride	6.65	6.68	-0.03
Acetylcyanide	6.45	6.38	0.07
Acetylhexane	14.83	14.77	0.06
Acetylmesitylene	19.96	20.08	-0.12
Acrylic acid	6.91	6.87	0.04
Acrylic acid chloride	8.40	8.40	0.00
Adamantane	16.51	16.59	-0.08
Adiponitrile	11.63	11.69	-0.06
Allicin	18.73	18.65	0.08
Allyl 2-furancarboxylate	15.76	15.49	0.27
Allyl acetate	10.48	10.60	-0.12
Allyl alcohol	6.73	6.79	-0.06
Allyl benzoate	18.43	18.50	-0.07
Allyl bromide	9.57	9.30	0.27
Allyl butyrate	14.14	14.27	-0.13
Allyl chloride	8.11	8.13	-0.02
Allyl chloroformate	10.69	10.75	-0.06
Allyl cyanide	7.83	7.98	-0.15
Allyl ether	11.83	12.28	-0.45

Allyl ethyl ether	10.53	10.57	-0.04
Allyl glycidyl ether	12.13	12.23	-0.10
Allyl iodide	11.55	11.34	0.21
Allyl methacrylate	14.01	14.17	-0.16
Allyl methyl ether	8.55	8.72	-0.17
Allyl phenyl ether	16.54	16.66	-0.12
Allyl propanoate	12.28	12.43	-0.15
Allyl sulfide	14.67	14.75	-0.08
Allyl trans-cinnamate	21.99	22.09	-0.10
Allyl vinyl ether	10.37	10.29	0.08
Allylacetoacetate	14.32	14.37	-0.05
Allylacrylate	12.21	12.31	-0.10
Allylamine	7.56	7.59	-0.03
Allylchlorodimethylsilane	15.06	15.34	-0.28
Allylcyclopentane	14.55	14.54	0.01
Allyldiethylamine	15.22	15.09	0.13
Allyldimethylamine	11.56	11.45	0.11
Allylmethyldichlorosilane	15.12	15.26	-0.14
Allyltrichlorosilane	15.45	15.19	0.26
Allyltriethoxysilane	22.09	22.00	0.09
Allyltrimethylsilane	15.52	15.55	-0.03
alpha-(Chloromethyl)benzenemethanol	16.64	16.72	-0.08
alpha,alpha-Dichloroacetoacetic acid ethylester	16.37	16.48	-0.11
alpha,alpha-Dichloroacetophenone	18.31	18.19	0.12
alpha,alpha-Dimethylacetoacetic acid ethylester	16.17	16.32	-0.15
alpha-Allylbenzenemethanol	18.04	18.37	-0.33
alpha-Bromoacetoacetic acid ethylester	15.97	15.75	0.22
alpha-Chloroacetoacetic acid ethylester	14.48	14.55	-0.07
alpha-Chlorobenzeneacetyl chloride	18.16	18.31	-0.15
alpha-Chlorohydrin	9.41	9.38	0.03
alpha-Chlorostyrene	16.17	16.08	0.09
alpha-Curcumene	26.74	27.11	-0.37
alpha-D-Glucose	14.28	14.43	-0.15
alpha-Ethylstyrene	18.21	17.83	0.38
alpha-Humulene	26.93	27.34	-0.41
alpha-Ionol	24.32	24.27	0.05
alpha-Ionone	24.28	23.81	0.47
alpha-Irone	25.80	25.63	0.17
alpha-Linolenic acid	34.21	34.28	-0.07
alpha-Methyl benzylamine	15.64	15.59	0.05
alpha-Methyl-2-furanmethanol	11.81	11.81	0.00
alpha-Methyl-4-isopropylbenzenepropanal	23.72	23.68	0.04



alpha-Methyl-4-morpholineethanol	15.61	15.59	0.02
alpha-Methylbenzeneacetaldehyde	15.96	16.28	-0.32
alpha-Methylbenzeneacetic acid	16.55	16.71	-0.16
alpha-Methylbenzenepropanol	18.20	18.49	-0.29
alpha-Methylcyclohexanemethanol	15.16	15.23	-0.07
alpha-Methylcyclopropanemethanol	10.05	9.72	0.33
alpha-Methylstyrene	16.11	15.99	0.12
alpha-Naphthaleneazide	21.01	21.11	-0.10
alpha-Pentylcinnamaldehyde	25.83	25.42	0.41
alpha-Phellandrene	17.95	18.19	-0.24
alpha-Phenylacetoacetic acid ethylester	22.81	22.74	0.07
alpha-Pinene	17.43	17.41	0.02
alpha-Santalol	26.65	26.28	0.37
alpha-Terpinene	18.22	18.23	-0.01
alpha-Terpineol	18.71	18.83	-0.12
alpha-Terpineol acetate	22.43	22.63	-0.20
alpha-Vetivone	26.94	26.69	0.25
Amyl acetate	14.36	14.39	-0.03
Amyl formate	12.59	12.61	-0.02
Amyl propionate	16.15	16.22	-0.07
Amyl thiocyanate	14.96	14.98	-0.02
Amylamine	11.41	11.38	0.03
Amylbenzene	19.71	19.76	-0.05
Amylobarbitone	22.80	22.72	0.08
Amylsilane	14.13	14.14	-0.01
Amylsulfinyl chloride	15.60	15.71	-0.11
Anabasine	19.39	19.31	0.08
Anatabine	19.04	19.23	-0.19
Angelic acid	10.71	10.61	0.10
Aniline	12.21	12.13	0.08
Anise alcohol	15.54	15.56	-0.02
Anisole	13.06	13.10	-0.04
Anisyl methyl ketone	18.66	18.78	-0.12
Anthracene	24.97	24.75	0.22
Apiole	23.89	23.56	0.33
Arachic alcohol	37.99	38.11	-0.12
Arachidic acid	38.45	38.19	0.26
Arecoline	16.85	16.84	0.01
Ascaridole	18.65	19.00	-0.35
Aspon	37.44	37.73	-0.29
Azepane	12.53	12.35	0.18
Azetidine	6.91	6.84	0.07

Azidobenzene	14.04	13.99	0.05
Azocane	14.02	14.18	-0.16
Azomethane	7.84	7.94	-0.10
Benzal bromide	18.72	18.48	0.24
Benzalaniline	23.68	23.40	0.28
Benzalchloride	16.15	16.25	-0.10
Benzaldehyde	12.81	12.63	0.18
Benzedrine	17.45	17.42	0.03
Benzene	10.41	10.51	-0.10
Benzeneazoethane	17.81	17.54	0.27
Benzenesulfonylchloride	16.26	16.17	0.09
Benzenethiol	13.66	13.68	-0.02
Benzhydryl chloride	23.95	24.04	-0.09
Benzo[a]phenanthrene	32.24	31.87	0.37
Benzo[b]furan	13.91	13.93	-0.02
Benzo[c]isoxazole	13.22	12.94	0.28
Benzo[d]isoxazole	12.96	13.05	-0.09
Benzonitrile	12.49	12.34	0.15
Benzophenone	22.47	22.26	0.21
Benzophenoneimine	23.24	23.43	-0.19
Benzophenone-N-methylimine	25.27	25.26	0.01
Benzotrifluoride	12.19	12.53	-0.34
Benzoxazole	12.98	13.35	-0.37
Benzoyl bromide	15.70	15.75	-0.05
Benzoyl chloride	14.73	14.58	0.15
Benzyl 3-methylbutanoate	22.01	22.27	-0.26
Benzyl acetate	16.66	16.78	-0.12
Benzyl acrylate	18.31	18.50	-0.19
Benzyl alcohol	12.90	12.98	-0.08
Benzyl benzoate	24.75	24.68	0.07
Benzyl butanoate	20.27	20.45	-0.18
Benzyl chloroacetate	18.86	18.69	0.17
Benzyl chloroformate	17.18	16.94	0.24
Benzyl ethyl ether	16.63	16.76	-0.13
Benzyl formate	15.07	15.00	0.07
Benzyl isobutyrate	20.05	20.44	-0.39
Benzyl isonitrile	14.51	14.37	0.14
Benzyl laurate	34.76	35.14	-0.38
Benzyl mercaptan	15.38	15.46	-0.08
Benzyl methacrylate	20.07	20.36	-0.29
Benzyl methyl ether	14.81	14.91	-0.10
Benzyl nitrite	14.85	14.84	0.01

Benzylamine	13.58	13.78	-0.20
Benzylbromide	15.59	15.49	0.10
Benzylcarbinol isobutyrate	22.03	22.27	-0.24
Benzylethylamine	17.21	17.43	-0.22
Benzylidene fluoride	12.20	12.38	-0.18
Benzylisopropylamine	19.59	19.23	0.36
Benzylisothiocyanate	18.11	18.22	-0.11
Benzylmethylamine	15.53	15.61	-0.08
Benzylmethylsulfide	17.29	17.31	-0.02
Benzylsalicylate	25.54	25.39	0.15
Benzyl-t-butanol	20.15	20.30	-0.15
Benzyltrimethylsilane	21.85	21.73	0.12
beta-Chlorostyrene	16.44	16.03	0.41
beta-Citronellol	19.71	19.69	0.02
beta-Cyclocitral	18.42	18.53	-0.11
beta-Elemene	26.93	27.18	-0.25
beta-Farnesene	28.00	28.06	-0.06
beta-Ionol	24.38	24.31	0.07
beta-Methylbenzeneethanamine	17.43	17.43	0.00
beta-Methylbenzenepropanoic acid	18.36	18.54	-0.18
beta-Phellandrene	17.97	18.15	-0.18
beta-Santalol	26.86	27.05	-0.19
beta-Terpineol	18.76	18.78	-0.02
beta-Vetivone	26.77	26.69	0.08
Bicyclo[2.2.1]hept-5-ene-2-carbaldehyde	13.74	13.96	-0.22
Bicyclo[2.2.1]hept-5-ene-2-carbonitrile	13.64	13.67	-0.03
Bicyclohexane	21.10	21.14	-0.04
Bicyclopophosphate	12.87	13.13	-0.26
Bicyclopophite	13.32	13.56	-0.24
Bicyclothiophosphate	15.74	16.11	-0.37
Bis(1-chloroethyl)ether	12.93	12.76	0.17
Bis(1-phenylethyl)amine	28.91	28.94	-0.03
Bis(2-bromoethyl) ether	14.98	15.00	-0.02
Bis(2-butoxyethyl)phosphite	28.71	28.66	0.05
Bis(2-chloroethoxy-2-ethyl) fumarate	29.58	29.33	0.25
Bis(2-chloroethoxy-2-ethyl) maleate	29.40	29.33	0.07
Bis(2-chloroethyl) ether	12.51	12.66	-0.15
Bis(2-chloroethyl)carbonate	15.06	15.10	-0.04
Bis(2-cyanoethyl) ether	12.36	12.36	0.00
Bis(2-ethoxyethyl)phosphite	21.35	21.32	0.03
Bis(2-ethylhexyl) adipate	42.60	42.58	0.02
Bis(2-ethylhexyl) azelate	47.68	48.09	-0.41

Bis(2-ethylhexyl) phosphite	34.56	34.63	-0.07
Bis(2-ethylhexyl) sebacate	49.93	49.92	0.01
Bis(2-furfuryl)amine	19.23	19.32	-0.09
Bis(2-heptoxyethyl)phosphite	39.80	39.67	0.13
Bis(2-hexoxyethyl)phosphite	36.12	36.00	0.12
Bis(2-hydroxyethyl) sulfide	12.51	12.45	0.06
Bis(2-hydroxyethyl)ammonium hexanoate	23.19	23.13	0.06
Bis(2-hydroxyethyl)methylamine	12.60	12.67	-0.07
Bis(2-hydroxyethyl)phosphine	13.50	13.34	0.16
Bis(2-mercaptoethyl) sulfide	17.64	17.41	0.23
Bis(2-methallyl) carbonate	18.75	18.45	0.30
Bis(2-methoxyethyl)phosphite	17.63	17.62	0.01
Bis(2-pentoxyethyl)phosphite	32.44	32.33	0.11
Bis(2-propoxyethyl)phosphite	25.04	24.99	0.05
Bis(2-tolyl)-N-ethylaminoborane	31.36	31.26	0.10
Bis(2-tolyl)-N-isobutylaminoborane	34.91	34.92	-0.01
Bis(2-tolyl)-N-methylaminoborane	29.33	29.44	-0.11
Bis(3-aminopropyl)amine	15.78	15.92	-0.14
Bis(3-chloropropyl) ether	16.35	16.34	0.01
Bis(4-tolyl) ether	24.90	24.83	0.07
Bis(allylamino)borane	16.21	16.38	-0.17
Bis(butoxy fluoro oxophosphorus) oxide	23.24	23.21	0.03
Bis(butylamino)borane	20.31	20.30	0.01
Bis(butylthio) 2-(diethylmethylsilyl)ethyl borane	40.34	40.54	-0.20
Bis(butylthio) hexyl borane	35.11	34.95	0.16
Bis(butylthio) octyl borane	38.97	38.62	0.35
Bis(butylthio)borane	23.85	23.89	-0.04
Bis(chlorofluorooxophosphorus) oxide	11.37	11.19	0.18
Bis(chloromethyl)ether	8.99	8.97	0.02
Bis(cyclohexyl)amine	22.55	22.46	0.09
Bis(diallylamino)borane	26.89	27.24	-0.35
Bis(diethyl)disiloxane	23.21	23.19	0.02
Bis(diethylamino fluoro oxophosphorus) oxide	24.49	24.44	0.05
Bis(diethylamino fluoro thiophosphorus) oxide	30.43	30.34	0.09
Bis(diethylamino)borane	20.43	20.39	0.04
Bis(diethylmethylsilyl)amine	27.45	27.58	-0.13
Bis(diethylsilyl)amine	24.34	24.28	0.06
Bis(di-isoamylamino)borane	42.46	42.35	0.11
Bis(diisobutylamino)borane	34.99	35.01	-0.02
Bis(dimethylamino)bis(diethylamino)silane	31.51	31.46	0.05
Bis(dimethylphenylsilyl)amine	36.10	36.10	0.00
Bis(ethoxy fluoro oxophosphorus) oxide	15.89	15.86	0.03

Bis(ethyldimethylsilyl)amine	24.18	23.96	0.22
Bis(ethylisobutyl)disiloxane	30.50	30.50	0.00
Bis(ethylphenyl)disiloxane	35.22	35.33	-0.11
Bis(ethylthio) butylborane	23.86	23.93	-0.07
Bis(ethylthio) isobutylborane	23.90	23.92	-0.02
Bis(ethylthio) isopropylborane	21.94	22.11	-0.17
Bis(ethylthio) octyl borane	31.22	31.28	-0.06
Bis(ethylthio) propylborane	22.06	22.10	-0.04
Bis(ethylthio)borane	16.32	16.55	-0.23
Bis(fluoro phenoxy oxophosphorus) oxide	27.72	27.69	0.03
Bis(isobutyl) cyclohexylboronate	28.72	28.59	0.13
Bis(isopropylthio)borane	20.25	20.21	0.04
Bis(methoxy fluoro oxophosphorus) oxide	12.18	12.17	0.01
Bis(methylthio)methane	12.51	12.39	0.12
Bis(propylthio)borane	20.13	20.22	-0.09
Bis(t-butylthio)borane	24.49	24.18	0.31
Bis(trichlorosilyl)methane	20.25	20.50	-0.25
Bis(triethylsilyl)amine	31.05	31.20	-0.15
Bis(trihexylsilyl)acetylene	76.86	76.81	0.05
Bis(trimethoxysilyl)amine	22.32	22.35	-0.03
Bis(trimethoxysilylamino)dimethylsilane	30.76	30.78	-0.02
Bis(trimethylsilylamino)dimethylsilane	28.47	28.76	-0.29
Bis-N-(2-hydroxyethyl)-2-furfurylamine	19.15	19.39	-0.24
Bornyl acetate	21.81	21.84	-0.03
Brassic acid	41.80	41.78	0.02
Bromal	14.17	14.21	-0.04
Bromo butylthio isopentylborane	25.37	25.35	0.02
Bromo ethylthio isopentylborane	21.61	21.68	-0.07
Bromo ethylthio isopropylborane	17.85	18.04	-0.19
Bromo ethylthio phenylborane	22.70	22.46	0.24
Bromo-2-chlorobenzene	15.43	15.43	0.00
Bromoacetic acid	8.10	8.22	-0.12
Bromoacetone	9.27	9.53	-0.26
Bromoacetyl bromide	10.94	10.92	0.02
Bromobenzene	13.46	13.52	-0.06
Bromochloroacetic acid	10.21	10.10	0.11
Bromocycloheptane	15.77	15.94	-0.17
Bromocyclohexane	14.13	14.10	0.03
Bromocyclopentane	12.28	12.26	0.02
Bromoethane	7.55	7.59	-0.04
Bromoethylene	7.45	7.38	0.07
Bromomethylether	8.43	8.71	-0.28

Bromopentafluorobenzene	13.26	13.32	-0.06
Bromotriethylsilane	18.41	18.47	-0.06
Bromotrimethylsilane	13.05	13.04	0.01
Butadiyne	6.80	6.57	0.23
Butanal	8.34	8.40	-0.06
Butanal oxime	9.93	9.98	-0.05
Butanamide	9.64	9.44	0.20
Butane	8.20	8.19	0.01
Butane-1,2,4-triol	9.93	9.87	0.06
Butane-2,3-dinitrite	13.17	13.03	0.14
Butanedial	8.21	8.60	-0.39
Butanedioic acid	9.54	9.46	0.08
Butanoic acid	8.80	8.82	-0.02
Butanoic anhydride	15.97	16.24	-0.27
Butanoyl chloride	10.23	10.35	-0.12
Buthiobate	46.25	46.20	0.05
Butoxy chloro phenylborine	22.42	22.29	0.13
Butoxyacetylene	11.67	11.76	-0.09
Butoxybenzene	18.63	18.61	0.02
Butoxytrimethylsilane	17.79	17.81	-0.02
Butyl 1-naphthaleneacetate	29.29	29.41	-0.12
Butyl 1-naphthoate	27.72	27.57	0.15
Butyl 1-naphthylketone	27.00	26.99	0.01
Butyl 2-(2,3-dihydroxypropoxy)ethyl thioether	22.25	22.30	-0.05
Butyl 2-hydroxybenzoate	21.52	21.16	0.36
Butyl 2-methylbutyrate	18.16	18.04	0.12
Butyl 2-naphthaleneacetate	29.42	29.41	0.01
Butyl 2-thiophenecarboxylate	20.05	19.85	0.20
Butyl 4-methylpentoxy dithiophosphinic acid	29.54	29.52	0.02
Butyl 4-oxopentanoate	18.08	18.17	-0.09
Butyl 4-toluenesulfonate	23.72	23.70	0.02
Butyl butanoate	16.19	16.22	-0.03
Butyl butoxy chloroborine	19.59	19.69	-0.10
Butyl butylxanthate	24.60	24.55	0.05
Butyl caproate	19.77	19.90	-0.13
Butyl chlorofluorophosphate	13.43	13.72	-0.29
Butyl chloroformate	12.53	12.71	-0.18
Butyl cyanoacetate	14.15	14.31	-0.16
Butyl cyclohexyloxy dithiophosphinic acid	28.69	28.69	0.00
Butyl dibutoxyborine	25.71	25.79	-0.08
Butyl dichloro phosphorus thioxide	18.71	18.71	0.00
Butyl diethyl phosphine oxide	18.92	18.91	0.01

Butyl enanthate	21.65	21.73	-0.08
Butyl ethoxy dithiophosphinic acid	22.17	22.19	-0.02
Butyl ethoxyethoxy dithiophosphinic acid	26.62	26.53	0.09
Butyl ethoxyethoxy S-(2-cyanoethyl) dithiophosphinate	31.66	31.80	-0.14
Butyl ethyl carbonate	14.93	14.97	-0.04
Butyl ethyl sulfide	15.02	15.00	0.02
Butyl ethylxanthate	20.88	20.88	0.00
Butyl fluorophosphoric acid	12.36	12.21	0.15
Butyl hydrocinnamate	23.97	24.12	-0.15
Butyl hydroperoxide	9.61	9.67	-0.06
Butyl isocyanate	10.97	11.00	-0.03
Butyl isopropoxy dithiophosphinic acid	23.89	24.03	-0.14
Butyl methoxy dithiophosphinic acid	20.43	20.34	0.09
Butyl N,N-diethylamino phosphorusoxy chloride	22.00	21.99	0.01
Butyl N,N-diethylamino phosphorusoxy fluoride	19.48	19.63	-0.15
Butyl octanoate	23.45	23.57	-0.12
Butyl pentanoate	17.95	18.06	-0.11
Butyl perfluorooctanoate	24.44	24.58	-0.14
Butyl phenyl sulfide	21.24	21.22	0.02
Butyl phenylacetate	22.15	22.29	-0.14
Butyl phosphorusoxy dichloride	15.41	15.42	-0.01
Butyl propanoate	14.33	14.39	-0.06
Butyl propyl carbonate	16.77	16.80	-0.03
Butyl ricinoleate	42.23	42.40	-0.17
Butyl thiocyanate	13.11	13.14	-0.03
Butyl trifluoroacetate	12.66	12.66	0.00
Butyl vinyl ether	12.27	12.25	0.02
Butylacetamide	13.40	13.20	0.20
Butylammonium nitrate	13.22	13.23	-0.01
Butylbenzene	17.88	17.93	-0.05
Butylcellosolve	13.20	13.09	0.11
Butylcyclohexane	18.58	18.34	0.24
Butylcyclopentane	16.53	16.50	0.03
Butyldi(3-acetoxypentyl)phosphine	31.94	32.10	-0.16
Butyldi(3-acetoxypentyl)phosphine thioxide	34.56	34.61	-0.05
Butyldi(3-aminopentyl)phosphine	26.06	26.10	-0.04
Butyldi(3-aminopentyl)phosphine thioxide	28.69	28.60	0.09
Butyldi(3-cyanopentyl)phosphine	26.79	26.88	-0.09
Butyldi(3-hydroxypentyl)phosphine	24.48	24.49	-0.01
Butyldi(3-hydroxypentyl)phosphine thioxide	26.95	27.00	-0.05
Butyldichlorophosphine	15.52	15.80	-0.28

Butyldimethylamine	13.41	13.41	0.00
Butylethylamine	13.26	13.20	0.06
Butyliodoacetylene	15.99	16.11	-0.12
Butylisopropylether	14.28	14.37	-0.09
Butylisothiocyanate	14.09	13.99	0.10
Butylmethylketone	11.88	11.97	-0.09
Butylnitrate	11.23	11.21	0.02
Butylphenylboronic acid	19.84	20.14	-0.30
Butylphosphonyl difluoride	11.26	11.23	0.03
Butylsilane	12.25	12.30	-0.05
Butylsulfinyl chloride	13.93	13.88	0.05
Butylthiodiethylborane	20.69	20.69	0.00
Butyltrichlorosilane	17.12	17.15	-0.03
Butyltriisothiocyanatosilane	29.30	29.23	0.07
Butyric acid methylester	10.63	10.71	-0.08
Butyrolin	16.36	16.20	0.16
Butyronitrile	8.07	8.11	-0.04
Butyrophenone	18.09	18.03	0.06
Camphene	17.24	17.37	-0.13
Camphor	17.60	17.58	0.02
Capraldehyde	19.23	19.41	-0.18
Caproic aldehyde	11.65	12.07	-0.42
Caprolactone	11.54	11.71	-0.17
Caproic acid	19.66	19.71	-0.05
Caprylene	15.37	15.41	-0.04
Caprylic aldehyde	15.72	15.74	-0.02
Caprylonitrile	15.45	15.45	0.00
Carbitol	13.90	13.76	0.14
Carbitol acetate	17.56	17.56	0.00
Carbon suboxide	6.55	6.57	-0.02
Carbonyl dicyanide	6.72	6.29	0.43
Carvacrylmethylketone	22.15	21.83	0.32
Carvenone	18.47	18.38	0.09
Carvone	18.11	18.30	-0.19
Cedrene	25.56	25.72	-0.16
Cedrol	26.53	26.31	0.22
Cetane	30.16	30.21	-0.05
Cetene	30.09	30.09	0.00
Cetyl palmitate	60.45	60.27	0.18
Chloral	10.54	10.56	-0.02
Chlordimeform	22.62	22.47	0.15
Chloro 2-octoxy phenylborine	29.50	29.63	-0.13



Chloro di(1,2,2-trimethylpropoxy)borine	27.47	27.49	-0.02
Chloro di(2-octoxy)borine	34.62	34.85	-0.23
Chloro di(sec-butoxy)borine	20.09	20.17	-0.08
Chloro dibutoxyborine	20.23	20.16	0.07
Chloro diisobutoxyborine	19.96	20.13	-0.17
Chloro dineopentoxyborine	23.92	23.82	0.10
Chloro dioctoxyborine	35.00	34.84	0.16
Chloro dipropoxyborine	16.58	16.49	0.09
Chloro(chloromethyl)dimethylsilane	13.65	13.68	-0.03
Chloro(dichloromethyl)dimethylsilane	15.61	15.63	-0.02
Chloro(methylthio)methane	9.70	9.49	0.21
Chloro-2,3-dinitrobenzene	17.98	17.71	0.27
Chloroacetic acid	6.96	7.06	-0.10
Chloroacetic acid ethylester	10.64	10.79	-0.15
Chloroacetone	8.51	8.36	0.15
Chloroacetone cyanohydrin	10.66	10.55	0.11
Chloroacetonitrile	6.35	6.34	0.01
Chloroacetyl chloride	8.52	8.59	-0.07
Chloroacetylene	6.07	5.86	0.21
Chlorobenzene	12.35	12.42	-0.07
Chlorocyclohexane	12.94	12.90	0.04
Chlorocyclopentane	11.11	11.06	0.05
Chlorodiethylsilane	13.84	13.76	0.08
Chlorodimethylphenylsilane	19.55	19.70	-0.15
Chlorodimethylsilane	10.27	10.13	0.14
Chloroethane	6.46	6.42	0.04
Chloroethyldimethylsilane	13.93	13.63	0.30
Chloroethylene	6.15	6.26	-0.11
Chloroethylene carbonate	8.74	8.73	0.01
Chloromethyl methyl ether	7.25	7.07	0.18
Chloromethylacetate	8.91	8.94	-0.03
Chloromethylchloroformate	8.96	9.09	-0.13
Chloromethylphenylsilane	18.02	18.01	0.01
Chloromethylsulfonyl fluoride	8.19	8.41	-0.22
Chloroprene	10.02	9.89	0.13
Chloroprotham	22.48	22.23	0.25
Chlorotriethylsilane	17.26	17.26	0.00
Chlorotrimethylsilane	11.84	11.82	0.02
Chlorovinyl dimethylsilane	13.67	13.48	0.19
Chlorthion	26.79	26.43	0.36
cis- Cyclooctene	14.38	14.60	-0.22
cis-(1-Methyl-1-propenyl)benzene	17.89	17.87	0.02

cis,trans,trans-1,5,9-Cyclododecatriene	21.51	21.79	-0.28
cis-1,2,3,5,6,8a-Hexahydro-4,7-dimethyl-1-isopropylnaphthalene	26.40	26.56	-0.16
cis-1,2-Bis(trimethylsilyl)-3,3-dichlorocyclopropane	28.29	27.99	0.30
cis-1,2-Dibromoethylene	10.16	10.42	-0.26
cis-1,2-Dichlorocyclohexane	14.76	14.79	-0.03
cis-1,2-Dichloroethylene	8.03	8.16	-0.13
cis-1,2-Dimethylcyclohexane	14.61	14.65	-0.04
cis-1,2-Dimethylcyclopentane	12.88	12.82	0.06
cis-1,2-Dimethylcyclopropane	9.41	9.14	0.27
cis-1,2-Dis(trimethylsilyl)-ethylene	22.94	23.01	-0.07
cis-1,2-Divinylcyclobutane	14.56	14.41	0.15
cis-1,3-Dichloro-2-butene	11.99	11.96	0.03
cis-1,3-Dichloropropene	9.99	10.08	-0.09
cis-1,3-Dimethylcyclohexane	14.79	14.65	0.14
cis-1,3-Dimethylcyclopentane	13.00	12.82	0.18
cis-1,3-Pentadiene	10.22	9.82	0.40
cis-1,4-Dichloro-2-butene	12.03	11.92	0.11
cis-1,4-Dimethylcyclohexane	14.47	14.65	-0.18
cis-1,4-Hexadiene	11.48	11.66	-0.18
cis-1-Bromo-1-butene	10.92	11.10	-0.18
cis-1-Bromopropene	9.12	9.26	-0.14
cis-1-Chloro-1-butene	9.84	9.97	-0.13
cis-1-Chloropropene	7.96	8.13	-0.17
cis-1-Ethyl-2-methylcyclopentane	14.62	14.65	-0.03
cis-1-Ethyl-3-methylcyclopentane	14.58	14.65	-0.07
cis-1-Methyl-2-propylcyclopentane	16.55	16.49	0.06
cis-1-Methyl-4-isopropylcyclohexane	18.34	18.31	0.03
cis-1-Phenyl-1-propene	16.22	16.01	0.21
cis-2,2,5,5-Tetramethyl-3-hexene	19.19	19.11	0.08
cis-2,2-Dimethyl-3-hexene	15.55	15.44	0.11
cis-2,3-Epoxybutane	8.05	8.02	0.03
cis-2,4,6-Trimethyl-1,3,5-trioxane	12.91	12.83	0.08
cis-2-Bromo-2-butene	10.99	11.05	-0.06
cis-2-Butene-1,4-diol	9.24	9.23	0.01
cis-2-Chloro-2-butene	9.91	10.06	-0.15
cis-2-Heptene	13.51	13.62	-0.11
cis-2-Hexen-1-ol	12.34	12.34	0.00
cis-2-Hexene	11.80	11.78	0.02
cis-2-Methoxy-4-(1-propenyl)phenol	19.78	19.30	0.48
cis-2-Methyl-1,3-pentadiene	12.16	11.69	0.47
cis-2-Methyl-3-hexene	13.70	13.60	0.10

cis-2-Methylcyclohexanol	13.34	13.39	-0.05
cis-2-Methylcyclopentanol	11.38	11.56	-0.18
cis-2-Octene	15.38	15.45	-0.07
cis-2-Penten-1-ol	10.45	10.50	-0.05
cis-2-Pentene	9.89	9.95	-0.06
cis-3,3,5-Trimethylcyclohexanol	16.99	17.06	-0.07
cis-3,4-Dimethyl-2-pentene	13.61	13.63	-0.02
cis-3,7-Dimethyl-2,6-octadien-1-ol acetate	23.19	23.46	-0.27
cis-3-Heptene	13.60	13.62	-0.02
cis-3-Hexen-1-ol	12.29	12.34	-0.05
cis-3-Hexenal	11.78	11.99	-0.21
cis-3-Hexene	11.79	11.78	0.01
cis-3-Methyl-2-heptene	15.50	15.48	0.02
cis-3-Methyl-2-hexene	13.62	13.64	-0.02
cis-3-Methyl-3-hexene	13.70	13.64	0.06
cis-3-Methylcyclohexanol	13.42	13.39	0.03
cis-3-Octene	15.51	15.45	0.06
cis-3-Penten-1-yne	9.40	9.14	0.26
cis-3-Phenyl-2-propen-1-ol	17.00	16.57	0.43
cis-4,4-Dimethyl-2-pentene	13.65	13.61	0.04
cis-4-Methyl-2-hexene	13.65	13.60	0.05
cis-4-Methylcyclohexanol	13.43	13.39	0.04
cis-4-Octene	15.44	15.45	-0.01
cis-4-Undecene	20.96	20.96	0.00
cis-5-Decene	19.13	19.12	0.01
cis-5-Methyl-2-hexene	13.66	13.60	0.06
cis-5-Undecene	20.97	20.96	0.01
cis-9-Octadecenitrile	33.56	33.72	-0.16
cis-alpha-Bisabolene	26.91	27.32	-0.41
cis-Benzaldehyde oxime	14.60	14.21	0.39
cis-Chlorobromoethylene	9.19	9.29	-0.10
cis-Crotyl alcohol	8.60	8.67	-0.07
cis-Cyclohexyl-1,2-diamine	13.77	13.68	0.09
cis-Decalin	17.40	17.47	-0.07
cis-Nerolidol	29.02	28.69	0.33
cis-Tetrahydro-2,5-dimethylthiophene	14.19	14.14	0.05
cis-Verbenol	18.09	17.98	0.11
Citronellal	19.17	19.34	-0.17
Citronellene	18.86	19.01	-0.15
Colamine	6.44	6.44	0.00
Coprostane	46.88	46.88	0.00
Crotonaldehyde	8.54	8.32	0.22

Crotonic acid	9.09	8.74	0.35
Crotonic acid anhydride	16.53	16.08	0.45
Cumene	15.98	16.07	-0.09
Cumic alcohol	18.47	18.54	-0.07
Cumylamine	17.24	17.42	-0.18
Cuscohygrine	26.10	26.12	-0.02
Cyanamide	3.44	3.69	-0.25
Cyanoacetylene	5.83	5.46	0.37
Cyanoethylene	6.24	6.15	0.09
Cyanogen	4.48	4.35	0.13
Cyclobutane	7.23	7.34	-0.11
Cyclobutanecarboxylic acid	9.87	9.80	0.07
Cyclobutanol	8.13	7.90	0.23
Cyclobutanone	7.39	7.45	-0.06
Cyclobutylamine	8.86	8.67	0.19
Cyclobutylphenylketone	19.27	19.00	0.27
Cyclodecane	18.22	18.35	-0.13
Cyclodecanol	18.73	18.92	-0.19
Cyclodecanone	18.01	18.46	-0.45
Cyclododecanone	21.73	22.13	-0.40
Cyclogeraniolane	16.85	16.49	0.36
Cycloheptane	12.76	12.85	-0.09
Cycloheptanol	13.34	13.41	-0.07
Cycloheptene	12.58	12.77	-0.19
Cyclohexane	10.99	11.01	-0.02
Cyclohexanecarbonitrile	12.67	12.75	-0.08
Cyclohexanecarbonyl chloride	14.82	15.00	-0.18
Cyclohexanecarboxaldehyde	13.22	13.04	0.18
Cyclohexanecarboxylic acid	13.29	13.47	-0.18
Cyclohexaneethanol	15.20	15.23	-0.03
Cyclohexanemethanamine	14.21	14.19	0.02
Cyclohexanemethanol	13.45	13.39	0.06
Cyclohexanethiol	14.14	14.05	0.09
Cyclohexanol	11.56	11.57	-0.01
Cyclohexanone	11.05	11.12	-0.07
Cyclohexene	10.72	10.93	-0.21
Cyclohexyl acetate	15.41	15.38	0.03
Cyclohexyl acrylate	17.32	17.09	0.23
Cyclohexyl benzoate	23.61	23.28	0.33
Cyclohexyl formate	13.39	13.60	-0.21
Cyclohexyl iodide	16.27	16.25	0.02
Cyclohexyl isothiocyanate	16.92	16.79	0.13

Cyclohexyl methacrylate	18.90	18.96	-0.06
Cyclohexyl propanoate	17.45	17.22	0.23
Cyclohexyl thiocyanate	15.97	15.96	0.01
Cyclohexylacetic acid	15.29	15.30	-0.01
Cyclohexylamine	12.41	12.34	0.07
Cyclohexyldichloroborane	16.64	16.61	0.03
Cyclohexylhydroperoxide	12.48	12.50	-0.02
Cyclohexylideneacetonitrile	14.47	14.55	-0.08
Cyclohexylisocyanate	13.74	13.79	-0.05
Cyclohexylisopropylamine	17.45	17.80	-0.35
Cyclohexyloxytrimethylsilane	20.66	20.64	0.02
Cyclohexylphosphine	15.11	15.00	0.11
Cyclohexyltrifluorosilane	13.58	13.62	-0.04
Cyclononane	16.40	16.52	-0.12
Cyclononanone	16.31	16.63	-0.32
Cyclooctane	14.56	14.68	-0.12
Cyclooctanol	15.01	15.25	-0.24
Cyclooctanone	14.55	14.79	-0.24
Cyclooctatetraene	14.03	14.37	-0.34
Cyclooctyne	14.16	14.09	0.07
Cyclopentadecane	27.27	27.53	-0.26
Cyclopentadecanone	27.58	27.64	-0.06
Cyclopentadiene	8.68	9.02	-0.34
Cyclopentane	9.17	9.18	-0.01
Cyclopentanecarbonitrile	10.92	10.91	0.01
Cyclopentanecarboxaldehyde	11.01	11.20	-0.19
Cyclopentanecarboxylic acid	11.62	11.63	-0.01
Cyclopentanemethanol	11.61	11.56	0.05
Cyclopentanepropanoic acid	15.20	15.30	-0.10
Cyclopentanol	9.73	9.74	-0.01
Cyclopentanone	9.20	9.28	-0.08
Cyclopentene	8.90	9.10	-0.20
Cyclopentyl acetate	13.51	13.54	-0.03
Cyclopentyl formate	11.71	11.76	-0.05
Cyclopentyl methyl ether	11.66	11.67	-0.01
Cyclopentylacetic acid	13.43	13.47	-0.04
Cyclopentylamine	10.89	10.51	0.38
Cyclopentylbenzene	18.86	18.90	-0.04
Cyclopentylphosphine	13.27	13.16	0.11
Cyclopropanecarbonitrile	7.57	7.24	0.33
Cyclopropanecarboxaldehyde	7.65	7.53	0.12
Cyclopropanecarboxylic acid	8.25	7.96	0.29

Cyclopropyl methyl ether	8.18	8.00	0.18
Cyclopropylamine	6.96	6.84	0.12
Cyclopropylbenzene	15.50	15.23	0.27
Cyclopropylcyclohexane	15.99	15.64	0.35
Cytosine	10.30	10.39	-0.09
DBCP	14.33	14.41	-0.08
Decahydro-2-naphthol	18.03	18.04	-0.01
Decamethylcyclopentasiloxane	37.00	36.96	0.04
Decamethyltetrasiloxane	34.16	34.19	-0.03
Decane	19.19	19.20	-0.01
Decanedioic acid	20.41	20.47	-0.06
Decanedioyl dichloride	23.52	23.53	-0.01
Decanenitrile	19.13	19.12	0.01
Decanoyl chloride	21.72	21.37	0.35
Decyl decanoate	38.20	38.25	-0.05
Decyl thiocyanate	24.16	24.16	0.00
Decyl vinyl ether	23.46	23.26	0.20
Decylbenzene	28.91	28.94	-0.03
Decylcyclohexane	29.40	29.35	0.05
Decylcyclopentane	27.54	27.51	0.03
Decyldiphenylnonylsilane	58.94	58.94	0.00
Decyldiphenylsilane	42.31	42.43	-0.12
Decyloxytrimethylsilane	28.82	28.82	0.00
DEET	23.19	23.16	0.03
DEHP	45.10	45.05	0.05
Demanyl phosphate	14.26	14.42	-0.16
Di(2-chloroethyl) chloromaleate	22.80	22.59	0.21
Di(2-ethylhexyl) fumarate	39.12	38.83	0.29
Di(2-ethylhexyl) maleate	38.79	38.83	-0.04
Di(cyclohexyloxy)dimethylsilane	29.34	29.26	0.08
Di-2-propenyldiethyleneglycol	20.91	21.01	-0.10
Di-3-tolylphosphorous aziridide	33.13	33.06	0.07
Di-3-tolylthiophosphoric aziride	35.32	35.27	0.05
Di-4-tolylphosphorous aziridide	33.16	33.06	0.10
Di-4-tolylthiophosphoric aziride	35.43	35.27	0.16
Diacetoxymethane	11.24	11.33	-0.09
Diacetyethylamine	13.67	13.30	0.37
Diallyl fumarate	20.04	20.26	-0.22
Diallyl maleate	20.18	20.26	-0.08
Diallyl oxalate	16.68	16.67	0.01
Diallyl succinate	20.16	20.34	-0.18
Diallylamine	12.78	12.95	-0.17

Diallyldimethylsilane	19.16	19.07	0.09
Diallylsulfoxide	15.08	15.10	-0.02
Diamyl isophthalate	34.17	34.07	0.10
Diamyl terephthalate	34.27	34.07	0.20
Diamylamine	20.61	20.54	0.07
Diamylsilane	23.23	23.21	0.02
Dibenzosuberone	25.32	25.23	0.09
Dibenzyl ether	24.66	24.66	0.00
Dibenzyl malonate	31.32	30.88	0.44
Dibenzylamine	25.16	25.33	-0.17
Dibromoacetonitrile	10.43	10.49	-0.06
Dibutoxy 2-hydroxyethoxy borine	23.58	23.26	0.32
Dibutoxy butyl phosphorus	27.61	27.43	0.18
Dibutoxymethane	18.76	18.62	0.14
Dibutoxyphosphinylsulfenyl chloride	25.10	25.09	0.01
Dibutoxythiophosphonate	22.35	22.60	-0.25
Dibutyl 3-oxo-2-butyl phosphate	28.03	27.79	0.24
Dibutyl adipate	27.91	27.93	-0.02
Dibutyl azodicarboxylate	22.94	23.09	-0.15
Dibutyl butanephosphonate	27.10	27.05	0.05
Dibutyl butylamino thiophosphate	31.33	31.37	-0.04
Dibutyl carbonate	18.57	18.64	-0.07
Dibutyl chloromaleate	26.31	26.13	0.18
Dibutyl decanedioate	35.16	35.27	-0.11
Dibutyl decanephosphonate	37.86	38.06	-0.20
Dibutyl dodecanephosphonate	41.64	41.73	-0.09
Dibutyl ether	16.26	16.20	0.06
Dibutyl ethylphosphonate	23.38	23.38	0.00
Dibutyl fumarate	24.54	24.18	0.36
Dibutyl heptanephosphonate	32.51	32.55	-0.04
Dibutyl hexadecanephosphonate	48.88	49.07	-0.19
Dibutyl hexanephosphonate	30.63	30.72	-0.09
Dibutyl isophthalate	30.54	30.40	0.14
Dibutyl maleate	24.18	24.18	0.00
Dibutyl malonate	22.37	22.42	-0.05
Dibutyl nonanephosphonate	36.12	36.22	-0.10
Dibutyl O-butyl phosphorus oxide	26.65	26.80	-0.15
Dibutyl octadecanephosphonate	52.65	52.74	-0.09
Dibutyl octanephosphonate	34.36	34.39	-0.03
Dibutyl oxalate	20.70	20.59	0.11
Dibutyl pentanephosphonate	28.81	28.88	-0.07
Dibutyl phosphite	19.86	19.98	-0.12

Dibutyl phthalate	30.54	30.40	0.14
Dibutyl suberate	31.49	31.60	-0.11
Dibutyl succinate	24.18	24.26	-0.08
Dibutyl tartrate	25.37	25.39	-0.02
Dibutyl terephthalate	30.65	30.40	0.25
Dibutyl tetradecanephosphonate	45.30	45.40	-0.10
Dibutyl thiophosphoryl chloride	24.90	24.77	0.13
Dibutylacetamide	20.66	20.69	-0.03
Dibutylamine	16.82	16.87	-0.05
Dibutylboronic anhydride	34.26	34.56	-0.30
Dibutylbutylaminoborane	26.04	25.92	0.12
Dibutyldiisothiocyanatosilane	30.83	30.86	-0.03
Dibutyldinonylsilane	52.14	52.30	-0.16
Dibutyldisulfide	21.87	21.92	-0.05
Dibutylethylthioborane	24.37	24.36	0.01
Dibutylmethylsilyl bromide	24.04	24.00	0.04
Dibutylnonylsilane	35.74	35.80	-0.06
Dibutylphenylaminoborane	28.75	28.77	-0.02
Dibutylphenylthioborane	30.31	30.45	-0.14
Dibutylphosphine	19.49	19.57	-0.08
Dibutylphosphinic chloride	19.35	19.34	0.01
Dibutylsilane	19.58	19.54	0.04
Dibutylsulfide	18.69	18.67	0.02
Dibutyltrisulfide	25.39	25.44	-0.05
Dichloro 4-chlorobutoxyborine	16.15	16.11	0.04
Dichloro butoxyborine	14.28	14.21	0.07
Dichloro isobutoxyborine	14.49	14.20	0.29
Dichloro neopentoxyborine	16.06	16.04	0.02
Dichloro octoxyborine	21.35	21.55	-0.20
Dichloro propoxyborine	12.14	12.38	-0.24
Dichloro(chloromethyl)methylsilane	13.54	13.59	-0.05
Dichloro(dichloromethyl)methylsilane	15.51	15.55	-0.04
Dichloroacetic acid	9.05	8.98	0.07
Dichloroacetonitrile	8.38	8.26	0.12
Dichloroacetyl chloride	10.43	10.51	-0.08
Dichlorodiethylsilane	15.34	15.36	-0.02
Dichlorodimethylsilane	11.75	11.74	0.01
Dichlorodiphenylsilane	27.74	27.50	0.24
Dichloromethylphenylsilane	19.35	19.62	-0.27
Dichloromethylphosphine	10.35	10.34	0.01
Dichlorophenylphosphine	17.97	17.98	-0.01
Dicosamethyldecasiloxane	78.29	78.55	-0.26



Dicyanomethane	6.22	6.19	0.03
Dicyclohexyl ether	22.02	21.85	0.17
Dicyclopropyl ketone	12.40	12.07	0.33
Didecyl isophthalate	52.61	52.42	0.19
Didecyldiphenylsilane	60.81	60.77	0.04
Diethanolamine	10.75	10.64	0.11
Diethoxy butyl phosphorus	20.39	20.09	0.30
Diethoxy ethyl phosphorus	16.70	16.42	0.28
Diethoxy fluorophosphate	12.26	12.39	-0.13
Diethoxy propyl phosphorus	18.53	18.25	0.28
Diethoxydimethylsilane	16.25	16.27	-0.02
Diethoxydiphenylsilane	32.14	32.03	0.11
Diethoxymethylphenylsilane	24.12	24.15	-0.03
Diethoxymethylsilane	14.60	14.54	0.06
Diethoxyphosphinylsulfenyl chloride	17.77	17.75	0.02
Diethyl 1,1-cyclobutanedicarboxylate	19.73	19.73	0.00
Diethyl 1-azepanyl thiophosphate	26.84	26.97	-0.13
Diethyl 2,2-diethylhydrazinosilane	21.97	22.14	-0.17
Diethyl 2,2-dimethylhydrazinosilane	18.39	18.50	-0.11
Diethyl 2-acetylsuccinate	20.68	20.68	0.00
Diethyl 2-aminomalonate	16.48	16.41	0.07
Diethyl 2-butylmalonate	22.45	22.41	0.04
Diethyl 2-methoxycarbonyl ethyl phosphine oxide	19.59	19.59	0.00
Diethyl 3-oxo-2-butyl phosphate	20.30	20.45	-0.15
Diethyl adipate	20.44	20.59	-0.15
Diethyl allylmalonate	20.33	20.45	-0.12
Diethyl azelate	25.98	26.10	-0.12
Diethyl azodicarboxylate	15.76	15.75	0.01
Diethyl benzylmalonate	26.53	26.64	-0.11
Diethyl bis(2,2-diethylhydrazino)silane	32.18	32.06	0.12
Diethyl bis(2,2-dimethylhydrazino)silane	24.76	24.78	-0.02
Diethyl bromomalonate	18.23	18.17	0.06
Diethyl butoxy phosphorus	19.94	19.93	0.01
Diethyl butylamino thiophosphate	23.97	24.03	-0.06
Diethyl cellosolve	13.29	13.20	0.09
Diethyl chloromalonate	16.64	16.97	-0.33
Diethyl cyclopropane-1,1-dicarboxylate	18.24	17.90	0.34
Diethyl decanedioate	27.85	27.93	-0.08
Diethyl decoxy phosphorus	30.95	30.94	0.01
Diethyl dibutylmalonate	29.74	29.76	-0.02
Diethyl dicarbonate	13.79	13.73	0.06
Diethyl diethylaminosilane	20.75	20.64	0.11

Diethyl disulfide	14.53	14.58	-0.05
Diethyl ethoxy phosphorus	16.26	16.26	0.00
Diethyl ethoxycarbonylmethyl phosphorus oxide	19.58	19.60	-0.02
Diethyl ethylidenemalonate	18.36	18.70	-0.34
Diethyl ethylmalonate	18.63	18.74	-0.11
Diethyl ethylphenylmalonate	28.26	28.48	-0.22
Diethyl ethylphosphonate	16.12	16.03	0.09
Diethyl fumarate	17.25	16.84	0.41
Diethyl glutaconate	18.58	18.67	-0.09
Diethyl glutarate	18.63	18.75	-0.12
Diethyl heptoxy phosphorus	25.44	25.43	0.01
Diethyl hexoxy phosphorus	23.60	23.60	0.00
Diethyl isobutoxy phosphorus	20.03	19.91	0.12
Diethyl isobutylmalonate	22.30	22.39	-0.09
Diethyl isophthalate	23.37	23.05	0.32
Diethyl isopropoxy phosphorus	18.15	18.10	0.05
Diethyl isopropylidenemalonate	20.69	20.57	0.12
Diethyl isopropylmalonate	20.32	20.56	-0.24
Diethyl itaconate	18.50	18.66	-0.16
Diethyl ketomalonate	15.65	15.19	0.46
Diethyl malate	17.41	17.48	-0.07
Diethyl maleate	16.93	16.84	0.09
Diethyl malonate	15.04	15.08	-0.04
Diethyl methylmalonate	16.83	16.90	-0.07
Diethyl methylphosphonate	14.36	14.25	0.11
Diethyl methylsuccinate	18.62	18.74	-0.12
Diethyl N,N-diethylamino phosphate	20.99	20.92	0.07
Diethyl nonoxy phosphorus	28.97	29.10	-0.13
Diethyl octoxy phosphorus	27.21	27.27	-0.06
Diethyl O-ethyl phospsphorus oxide	15.63	15.78	-0.15
Diethyl oxalate	13.31	13.25	0.06
Diethyl phenylmalonate	25.06	24.80	0.26
Diethyl phosphite	12.66	12.64	0.02
Diethyl phthalate	23.07	23.05	0.02
Diethyl propoxy phosphorus	18.04	18.09	-0.05
Diethyl propylmalonate	20.50	20.57	-0.07
Diethyl succinate	16.80	16.92	-0.12
Diethyl sulfate	12.61	12.62	-0.01
Diethyl sulfite	12.89	12.67	0.22
Diethyl sulphide	11.33	11.33	0.00
Diethyl tartrate	18.02	18.04	-0.02
Diethyl terephthalate	23.26	23.05	0.21

Diethyl thiodipropionate	23.29	23.73	-0.44
Diethyl thiophosphoryl chloride	17.32	17.43	-0.11
Diethyl xanthate	17.14	17.21	-0.07
Diethylacetaldehyde	11.94	12.05	-0.11
Diethylacetamide	13.11	13.35	-0.24
Diethylamine	9.66	9.53	0.13
Diethylamino ethyl fluorophosphate	16.62	16.68	-0.06
Diethylamino ethyl fluoroethiophosphate	19.45	19.63	-0.18
Diethylaminoacetone	15.19	15.32	-0.13
Diethylbutylthiophosphine	24.68	24.81	-0.13
Diethylcarbonate	11.31	11.30	0.01
Diethylcyanamide	11.35	11.28	0.07
Diethyldifluorosilane	11.00	11.03	-0.03
Diethyldiisothiocyanatosilane	23.61	23.51	0.10
Diethylene glycol dimethyl ether	13.96	13.85	0.11
Diethyleneglycol	10.04	9.98	0.06
Diethyleneglycol bischloroformate	17.85	17.90	-0.05
Diethyleneglycol diacetate	17.77	17.59	0.18
Diethyleneglycol diaminopropyl ether	23.98	23.93	0.05
Diethyleneglycol diethyl ether	17.64	17.54	0.10
Diethyleneglycol monobutyl ether	17.41	17.43	-0.02
Diethyleneglycol-di-n-butylether	24.93	24.88	0.05
Diethylketone	10.01	10.13	-0.12
Diethylmethylamine	11.59	11.56	0.03
Diethylmethylchlorosilane	15.31	15.44	-0.13
Diethylmethylsilanol	14.04	14.12	-0.08
Diethylnonylsilane	28.38	28.46	-0.08
Diethyloctylsilane	26.65	26.62	0.03
Diethylperoxide	9.84	9.82	0.02
Diethylphenyl 1-isopropoxyethoxysilane	31.82	31.76	0.06
Diethylphosphate	12.84	12.82	0.02
Diethylphosphine	12.14	12.22	-0.08
Diethylphosphinic chloride	12.07	12.00	0.07
Diethylpropylthiophosphine	21.05	21.14	-0.09
Diethylsilane	12.17	12.20	-0.03
Diethylsilanol	12.53	12.39	0.14
Diethyltrisulfide	17.99	18.10	-0.11
Difluoroacetic acid	5.33	5.11	0.22
Difluorodiphenylsilane	23.26	23.17	0.09
Difurfuryl ether	18.49	18.65	-0.16
Diglycidyl resorcinol ether	22.72	22.70	0.02
Diheptyl ether	27.28	27.21	0.07

Diheptyl ethylphosphonate	34.45	34.39	0.06
Diheptyl isophthalate	41.70	41.41	0.29
Diheptyl phosphite	30.99	30.99	0.00
Diheptyl sulfide	29.76	29.68	0.08
Dihexyl carbonate	26.04	25.98	0.06
Dihexyl disulfide	29.20	29.26	-0.06
Dihexyl ethylphosphonate	30.75	30.72	0.03
Dihexyl isophthalate	38.03	37.74	0.29
Dihexyl maleate	31.61	31.52	0.09
Dihexyl phosphite	27.25	27.32	-0.07
Dihexyl sulfide	26.06	26.01	0.05
Dihexyl terephthalate	37.82	37.74	0.08
Dihexylamine	24.25	24.21	0.04
Dihexylsulfate	27.35	27.30	0.05
Dihydro-2(3H)-thiophenone	10.48	10.62	-0.14
Dihydro-3-methyl-2(3H)-furanone	9.75	9.85	-0.10
Dihydro-3-methylene-2(3H)-furanone	9.59	9.78	-0.19
Dihydro-4-methyl-2(3H)-furanone	9.77	9.85	-0.08
Dihydrocarvone	18.22	18.33	-0.11
Dihydrolinalool	19.40	19.69	-0.29
Dihdropinene	17.74	17.45	0.29
Diisoamyl ether	19.92	19.84	0.08
Diisoamyl phthalate	34.23	34.03	0.20
Diisoamylbutylthioborane	31.71	31.67	0.04
Diisobutoxythiophosphonate	22.54	22.57	-0.03
Diisobutyl adipate	27.73	27.90	-0.17
Diisobutyl carbonate	18.61	18.61	0.00
Diisobutylamine	16.98	16.84	0.14
Diisobutylboronic anhydride	34.78	34.50	0.28
Diisobutylbutylthioborane	28.17	28.00	0.17
Diisobutylene	15.37	15.43	-0.06
Diisobutylphosphinic chloride	19.32	19.30	0.02
Diisobutylsulfite	20.04	19.98	0.06
Diisopentyl sulfide	22.40	22.31	0.09
Diisopentylamine	20.72	20.51	0.21
Diisopentylboronic anhydride	41.84	41.84	0.00
Diisopropoxyphosphinylsulfenyl chloride	21.40	21.43	-0.03
Diisopropyl adipate	24.38	24.27	0.11
Diisopropyl disulfide	18.31	18.24	0.07
Diisopropyl ether	12.61	12.54	0.07
Diisopropyl oxalate	17.07	16.93	0.14
Diisopropyl phthalate	27.02	26.73	0.29

Diisopropyl sulfide	15.29	14.99	0.30
Diisopropylamine	13.37	13.14	0.23
Diisopropylboronic anhydride	27.26	27.25	0.01
Diisopropylphosphinic chloride	15.59	15.72	-0.13
Dill-Apiole	23.48	23.56	-0.08
Dimethoxane	16.78	16.59	0.19
Dimethoxydiphenylsilane	28.42	28.33	0.09
Dimethoxymethane	7.58	7.58	0.00
Dimethyl 1,3-acetonedicarboxylate	15.46	15.17	0.29
Dimethyl 2-butyndioate	12.93	12.63	0.30
Dimethyl 2-methylsuccinate	14.93	15.04	-0.11
Dimethyl 3-oxo-2-butyl phosphate	16.58	16.76	-0.18
Dimethyl azelate	22.27	22.40	-0.13
Dimethyl bis(2,2-diethylhydrazino)silane	28.36	28.44	-0.08
Dimethyl bis(2,2-dimethylhydrazino)silane	21.22	21.16	0.06
Dimethyl bis(2-chloropropoxy)silane	23.72	23.71	0.01
Dimethyl butyl isopropylammonium bis(trifluoromethylsulfonyl)amide	31.24	31.34	-0.10
Dimethyl carbate	20.53	20.56	-0.03
Dimethyl carbonate	7.57	7.60	-0.03
Dimethyl chlorothiophosphate	13.72	13.74	-0.02
Dimethyl citraconate	15.03	15.01	0.02
Dimethyl cyclobutane-1,1-dicarboxylate	16.13	16.04	0.09
Dimethyl dipropylmalonate	22.23	22.39	-0.16
Dimethyl disulfide	10.84	10.74	0.10
Dimethyl ethylphosphonate	12.37	12.34	0.03
Dimethyl glutarate	14.90	15.06	-0.16
Dimethyl hexanedioate	16.77	16.89	-0.12
Dimethyl hexyl isopropylammonium bis(trifluoromethylsulfonyl)amide	35.34	35.01	0.33
Dimethyl isophthalate	19.50	19.36	0.14
Dimethyl itaconate	14.86	14.96	-0.10
Dimethyl maleate	13.01	13.14	-0.13
Dimethyl malonate	11.31	11.39	-0.08
Dimethyl methylmalonate	13.15	13.21	-0.06
Dimethyl oxalate	9.23	9.55	-0.32
Dimethyl phosphite	8.88	8.94	-0.06
Dimethyl phthalate	19.46	19.36	0.10
Dimethyl sebacate	24.13	24.24	-0.11
Dimethyl suberate	20.44	20.57	-0.13
Dimethyl succinate	13.09	13.22	-0.13
Dimethyl sulfate	8.84	8.92	-0.08

Dimethyl sulfide	7.71	7.49	0.22
Dimethyl sulfite	8.88	8.98	-0.10
Dimethyl sulfone	8.11	7.82	0.29
Dimethyl thiodipropionate	19.88	20.03	-0.15
Dimethylacetal	9.43	9.44	-0.01
Dimethylacetamide	9.60	9.71	-0.11
Dimethylamine	5.65	5.89	-0.24
Dimethylaminoacetaldehyde diethylacetal	18.00	18.35	-0.35
Dimethylcyanamide	7.82	7.64	0.18
Dimethyldi(2-ethylbutoxy)silane	31.03	30.92	0.11
Dimethyldi(2-octyloxy)silane	38.23	38.30	-0.07
Dimethyldi-2-butoxysilane	23.66	23.62	0.04
Dimethyldi-2-pentoxysilane	27.20	27.29	-0.09
Dimethyldiacetoxysilane	16.18	16.18	0.00
Dimethyldibutoxysilane	23.64	23.61	0.03
Dimethyldidodecyloxysilane	52.89	52.97	-0.08
Dimethyldiheptoxysilane	34.59	34.62	-0.03
Dimethyldihexoxysilane	30.71	30.95	-0.24
Dimethyldiisopropoxysilane	19.63	19.95	-0.32
Dimethyldiisothiocyanatosilane	19.79	19.89	-0.10
Dimethyldimethoxysilane	12.49	12.57	-0.08
Dimethyldinonyloxysilane	41.89	41.96	-0.07
Dimethyldioctoxysilane	38.25	38.29	-0.04
Dimethyldipentoxysilane	27.11	27.28	-0.17
Dimethyldiphenoxysilane	28.37	28.30	0.07
Dimethyldiphenylsilane	27.76	27.78	-0.02
Dimethyldipropoxysilane	20.19	19.94	0.25
Dimethylether	5.08	5.17	-0.09
Dimethylethylsilanol	12.21	12.30	-0.09
Dimethylketazine	14.28	14.29	-0.01
Dimethylperoxide	6.10	6.13	-0.03
Dimethylphenylsilane	17.85	18.06	-0.21
Dimethylphosphate	9.32	9.13	0.19
Dimethylphosphinic acid ethylester	12.12	12.22	-0.10
Dimethylpropylamine	11.35	11.57	-0.22
Dimethylpropylisopropylammonium bis(trifluoromethylsulfonyl)amide	29.16	29.50	-0.34
Dimethyltrisulfide	14.27	14.26	0.01
Dimethylvinylethoxysilane	15.78	15.80	-0.02
Di-n-butylsulfite	20.02	20.01	0.01
Di-n-hexylether	23.57	23.54	0.03
Di-n-octylether	30.96	30.88	0.08

Dinonyl ether	34.59	34.55	0.04
Dinonyl isophthalate	48.94	48.75	0.19
Dinonyldiphenylsilane	57.28	57.10	0.18
DINP	48.93	48.72	0.21
Di-n-propylmaleate	20.56	20.51	0.05
Di-n-propylsulfate	16.30	16.29	0.01
Di-n-propylsulfone	15.44	15.33	0.11
Diethyl butoxyborine	39.65	39.95	-0.30
Diethyl ethylphosphonate	38.13	38.06	0.07
Diethyl isophthalate	45.16	45.08	0.08
Diethyl maleate	38.88	38.86	0.02
Diethyl phosphite	34.63	34.66	-0.03
Diethyl sulfide	33.40	33.35	0.05
Diethyl terephthalate	45.28	45.08	0.20
Diethylamine	31.77	31.55	0.22
Dipentyl carbonate	22.27	22.31	-0.04
Dipentyl ethylphosphonate	27.06	27.05	0.01
Dipentyl phosphite	23.59	23.65	-0.06
Dipentyl sulfide	22.35	22.34	0.01
Diphenyl 2-ethylhexyl phosphate	39.42	39.49	-0.07
Diphenyl ether	21.03	21.02	0.01
Diphenyl fluorophosphate	23.90	24.22	-0.32
Diphenyl phosphonate	24.45	24.47	-0.02
Diphenyl sulfide	23.69	23.56	0.13
Diphenylacetaldehyde	23.80	24.18	-0.38
Diphenylketene	24.19	24.03	0.16
Diphenylmethane	22.02	22.15	-0.13
Diphenylmethylaniline	23.26	23.49	-0.23
Diphenylmethylsilane	25.88	25.94	-0.06
Diphenylmethylsilylamine	26.97	26.98	-0.01
Diphenylnonylsilane	40.55	40.60	-0.05
Diphenylphosphinic chloride	23.57	23.70	-0.13
Diphenylphosphorous aziridide	29.14	29.25	-0.11
Diphenylsilane	24.39	24.34	0.05
Diphenylthiophosphoric aziride	31.52	31.46	0.06
Dipropoxy butyl phosphorus	23.83	23.76	0.07
Dipropoxy propyl phosphorus	21.73	21.92	-0.19
Dipropoxymethane	15.02	14.95	0.07
Dipropoxyphosphinylsulfenyl chloride	21.40	21.42	-0.02
Dipropoxythiophosphonate	19.19	18.93	0.26
Dipropyl adipate	24.16	24.26	-0.10
Dipropyl azodicarboxylate	19.40	19.42	-0.02

Dipropyl butylphosphonate	23.55	23.38	0.17
Dipropyl carbonate	14.92	14.97	-0.05
Dipropyl disulfide	18.19	18.25	-0.06
Dipropyl ether	12.59	12.53	0.06
Dipropyl ethylphosphonate	19.72	19.71	0.01
Dipropyl fumarate	20.80	20.51	0.29
Dipropyl heptylphosphonate	29.08	28.88	0.20
Dipropyl hexylphosphonate	27.23	27.05	0.18
Dipropyl isophthalate	27.09	26.73	0.36
Dipropyl octylphosphonate	30.91	30.72	0.19
Dipropyl O-propyl phosphorus oxide	21.20	21.29	-0.09
Dipropyl oxalate	17.00	16.92	0.08
Dipropyl pentylphosphonate	25.39	25.21	0.18
Dipropyl phosphite	16.25	16.31	-0.06
Dipropyl propylphosphonate	21.76	21.54	0.22
Dipropyl succinate	20.46	20.59	-0.13
Dipropyl sulfide	15.44	15.00	0.44
Dipropyl terephthalate	27.02	26.73	0.29
Dipropylacetamide	16.70	17.02	-0.32
Dipropylamine	13.29	13.20	0.09
Dipropylbutylthioborane	24.38	24.36	0.02
Dipropyldifluorosilane	14.76	14.70	0.06
Dipropylene glycol monomethyl ether	15.62	15.59	0.03
Dipropylethylthioborane	20.80	20.69	0.11
Dipropylisobutylaminoborane	22.19	22.23	-0.04
Dipropylperoxide	13.49	13.49	0.00
Dipropylphenylaminoborane	25.10	25.10	0.00
Dipropylphenylthioborane	26.82	26.78	0.04
Dipropylphosphinic chloride	15.54	15.67	-0.13
Dipropylsilane	15.89	15.87	0.02
Dipropylsulfoxide	15.27	15.35	-0.08
Di-s-butylamine	17.07	16.81	0.26
Di-s-butylsulfide	18.69	18.66	0.03
Disilanomethane	10.77	10.81	-0.04
Di-t-amyl disulfide	25.71	25.88	-0.17
Di-t-amyl peroxide	20.83	20.80	0.03
Di-t-butyl ether	16.16	16.16	0.00
Di-t-butyl disulfide	22.15	22.21	-0.06
Di-t-butylsulfide	19.14	18.96	0.18
Di-t-butyltetrasulfide	29.33	29.25	0.08
Di-t-butyltrisulfide	25.66	25.73	-0.07
Divinyl ether	8.69	8.30	0.39



Divinyl sulfide	10.90	10.60	0.30
Divinyl sulfone	11.23	11.02	0.21
DMSO	8.00	7.84	0.16
Docosane	41.29	41.23	0.06
Dodecahydrosqualene	55.83	55.81	0.02
Dodecamethylcyclohexasiloxane	44.35	44.36	-0.01
Dodecamethylpentasiloxane	41.54	41.58	-0.04
Dodecane	22.84	22.87	-0.03
Dodecanedioic acid	24.09	24.14	-0.05
Dodecanoic anhydride	45.84	45.61	0.23
Dodecanoyl chloride	25.21	25.04	0.17
Dodecyl acetate	27.13	27.24	-0.11
Dodecyl thiocyanate	27.86	27.83	0.03
Dodecylcyclohexane	33.08	33.02	0.06
Dodecyloxirane	26.30	26.37	-0.07
DTBP	17.22	17.12	0.10
d-Verbenone	17.53	17.52	0.01
E-beta-Caryophyllene	26.19	26.50	-0.31
Eicosamethylnonasiloxane	71.07	71.15	-0.08
Eicosane	37.62	37.55	0.07
Elaidic acid	34.45	34.44	0.01
Enanthic acid	14.22	14.33	-0.11
Entprol	31.85	31.82	0.03
Epichlorohydrin	8.11	8.08	0.03
Eps-Chlorocapronitrile	13.69	13.68	0.01
Ethane	4.47	4.52	-0.05
Ethanediol diacetate	13.16	13.25	-0.09
Ethanesulfonic acid	8.51	8.73	-0.22
Ethanesulfonylchloride	10.15	10.01	0.14
Ethanethioic acid S-(1-methylheptyl) ester	22.60	22.47	0.13
Ethanol	5.12	5.08	0.04
Ethene	4.36	4.35	0.01
Ethoglucid	25.28	25.20	0.08
Ethoheptazine	30.39	30.30	0.09
Ethoxyacetaldehyde	8.90	9.07	-0.17
Ethoxyacetic acid	9.47	9.49	-0.02
Ethoxyacetylchloride	11.02	11.02	0.00
Ethoxyacetylene	8.15	8.09	0.06
Ethoxybenzene	14.95	14.94	0.01
Ethoxydichloromethylsulfenyl chloride	16.22	16.18	0.04
Ethoxytriethylsilane	19.46	19.57	-0.11
Ethoxytrihexylsilane	41.85	41.60	0.25

Ethoxytrimethylsilane	14.14	14.14	0.00
Ethyl (4-methoxyphenyl)acetate	20.91	21.20	-0.29
Ethyl (E)-3-chloro-2-butenolate	14.69	14.42	0.27
Ethyl (Z)-3-chloro-2-butenolate	14.64	14.42	0.22
Ethyl 10-undecenoate	25.37	25.28	0.09
Ethyl 1-naphthaleneacetate	25.58	25.74	-0.16
Ethyl 1-Naphthoate	23.97	23.90	0.07
Ethyl 1-piperidinepropanoate	20.60	20.56	0.04
Ethyl 2-(methoxyethyl)acetoacetate	18.90	18.81	0.09
Ethyl 2,3-dibromopropionate	16.89	16.87	0.02
Ethyl 2,3-dichloropropionate	14.64	14.51	0.13
Ethyl 2,4-dibromobutanoate	18.67	18.71	-0.04
Ethyl 2-acetyl-3-methylbutanoate	18.12	18.14	-0.02
Ethyl 2-acetyl-4-pentenoate	17.92	18.03	-0.11
Ethyl 2-acetylhexanoate	20.03	19.99	0.04
Ethyl 2-acetylpentanoate	18.09	18.15	-0.06
Ethyl 2-aminoacetate	10.16	10.24	-0.08
Ethyl 2-bromo-2-methylpropanoate	15.50	15.69	-0.19
Ethyl 2-bromo-3-methylbutyrate	17.44	17.46	-0.02
Ethyl 2-bromoacrylate	13.48	13.53	-0.05
Ethyl 2-bromobutyrate	15.58	15.64	-0.06
Ethyl 2-bromopropionate	13.62	13.81	-0.19
Ethyl 2-butynoate	12.08	11.96	0.12
Ethyl 2-chlorobutanoate	14.16	14.44	-0.28
Ethyl 2-chloropropionate	12.64	12.61	0.03
Ethyl 2-cyano-2-phenylacetate	20.26	20.36	-0.10
Ethyl 2-cyclopentanone-1-carboxylate	15.49	15.47	0.02
Ethyl 2-ethylacetoacetate	16.17	16.32	-0.15
Ethyl 2-ethylcaproate	19.80	19.88	-0.08
Ethyl 2-furancarboxylate	14.12	13.78	0.34
Ethyl 2-hydroxy-3-butenolate	12.88	12.99	-0.11
Ethyl 2-methoxybenzoate	19.60	19.37	0.23
Ethyl 2-methylacetoacetate	14.50	14.48	0.02
Ethyl 2-methylbenzoate	18.76	18.69	0.07
Ethyl 2-naphthaleneacetate	25.70	25.74	-0.04
Ethyl 2-naphthoate	24.19	23.90	0.29
Ethyl 2-picolinate	16.02	15.94	0.08
Ethyl 2-thiophenecarboxylate	16.32	16.18	0.14
Ethyl 3,5-dinitrobenzoate	22.11	22.07	0.04
Ethyl 3-aminobenzoate	18.08	18.40	-0.32
Ethyl 3-bromopropionate	13.70	13.79	-0.09
Ethyl 3-butenolate	12.30	12.43	-0.13

Ethyl 3-chlorobutanoate	14.13	14.44	-0.31
Ethyl 3-chloropropionate	12.50	12.62	-0.12
Ethyl 3-cyclohexene-1-carboxylate	17.21	17.12	0.09
Ethyl 3-ethoxypropionate	15.02	15.06	-0.04
Ethyl 3-hydroxybutyrate	12.99	13.12	-0.13
Ethyl 3-methyl-2-butenolate	14.40	14.34	0.06
Ethyl 3-oxopentanoate	14.38	14.50	-0.12
Ethyl 4-bromoacetoacetate	15.61	15.73	-0.12
Ethyl 4-bromobenzoate	19.99	19.79	0.20
Ethyl 4-bromobutyrate	15.52	15.62	-0.10
Ethyl 4-chloroacetoacetate	14.45	14.56	-0.11
Ethyl 4-chlorobutyrate	14.37	14.46	-0.09
Ethyl 4-fluorobenzoate	16.71	16.74	-0.03
Ethyl 4-methoxybenzoate	19.84	19.37	0.47
Ethyl 4-methyl-3-oxopentanoate	16.36	16.32	0.04
Ethyl 4-methylbenzoate	18.92	18.69	0.23
Ethyl 4-methylcaproate	17.66	18.04	-0.38
Ethyl 4-methylpentanoate	16.10	16.21	-0.11
Ethyl 4-pyridinecarboxylate	15.94	15.87	0.07
Ethyl 5-bromovalerate	17.16	17.46	-0.30
Ethyl 5-oxohexanoate	16.30	16.33	-0.03
Ethyl 6-bromohexanoate	19.44	19.29	0.15
Ethyl acetate	8.82	8.88	-0.06
Ethyl acetoacetate	12.51	12.66	-0.15
Ethyl acrylate	10.58	10.60	-0.02
Ethyl amyl ether	14.41	14.37	0.04
Ethyl benzoate	16.83	16.78	0.05
Ethyl bis(2,2-diethylhydrazino)silane	28.45	28.50	-0.05
Ethyl bis(2,2-dimethylhydrazino)silane	21.27	21.22	0.05
Ethyl bis(2-chloropropoxy)silane	23.68	23.80	-0.12
Ethyl bis(diethylamino)silane	25.47	25.48	-0.01
Ethyl bis(N,N-diethylamino) phosphate	25.37	25.40	-0.03
Ethyl bis(N,N-dimethylamino) phosphate	18.06	18.12	-0.06
Ethyl bromoacetate	11.81	11.95	-0.14
Ethyl but-3-yne- 1-carboxylate	13.50	13.58	-0.08
Ethyl butanoate	12.49	12.55	-0.06
Ethyl butylxanthate	21.27	20.88	0.39
Ethyl caprylate	19.86	19.90	-0.04
Ethyl chlorofluoroacetate	10.85	10.83	0.02
Ethyl chlorofluorophosphate	10.08	10.05	0.03
Ethyl chloroformate	9.13	9.04	0.09
Ethyl chlorohydroxyacetate	11.33	11.39	-0.06

Ethyl crotonate	12.59	12.47	0.12
Ethyl cyanoacetate	10.60	10.64	-0.04
Ethyl cyanoformate	9.11	8.80	0.31
Ethyl cyclohexylacetate	19.05	19.03	0.02
Ethyl cyclopropanecarboxylate	11.89	11.69	0.20
Ethyl decanoate	23.50	23.57	-0.07
Ethyl diacetylacetate	17.21	16.78	0.43
Ethyl dibromoacetate	15.14	14.94	0.20
Ethyl dichloroacetate	12.75	12.71	0.04
Ethyl diethoxyacetate	17.57	17.50	0.07
Ethyl diethylmalonate	22.69	22.42	0.27
Ethyl dodecanoate	27.20	27.24	-0.04
Ethyl elaidate	38.03	38.17	-0.14
Ethyl ethanethiolsulfinate	15.15	15.23	-0.08
Ethyl ether	8.92	8.86	0.06
Ethyl ethoxyacetate	13.20	13.22	-0.02
Ethyl ethylcarbamate	12.01	12.01	0.00
Ethyl fluoroacetate	8.83	8.85	-0.02
Ethyl fluorophosphoric acid	8.70	8.54	0.16
Ethyl formate	7.06	7.10	-0.04
Ethyl glycolate	9.40	9.44	-0.04
Ethyl heptafluorobutanoate	12.92	12.97	-0.05
Ethyl heptanoate	17.63	18.06	-0.43
Ethyl hexadecanoate	34.29	34.58	-0.29
Ethyl hexanoate	16.13	16.22	-0.09
Ethyl hexyl carbonate	18.62	18.64	-0.02
Ethyl hydrocinnamate	20.32	20.45	-0.13
Ethyl hydrogen succinate	13.12	13.19	-0.07
Ethyl hydroperoxide	6.11	6.00	0.11
Ethyl hydrosorbate	16.11	16.15	-0.04
Ethyl iodide	9.60	9.62	-0.02
Ethyl iodoacetate	13.91	13.99	-0.08
Ethyl isobutanoate	12.49	12.54	-0.05
Ethyl isobutyl 2-chloropropoxysilane	23.48	23.41	0.07
Ethyl isocrotonate	12.58	12.47	0.11
Ethyl isocyanate	7.24	7.33	-0.09
Ethyl isonitrile	6.54	6.47	0.07
Ethyl isothiocyanate	10.39	10.32	0.07
Ethyl isovalerate	14.33	14.37	-0.04
Ethyl lactate	11.29	11.28	0.01
Ethyl levulinate	14.39	14.50	-0.11
Ethyl linolenate	37.96	38.01	-0.05

Ethyl mercaptan	7.67	7.56	0.11
Ethyl mercaptoacetate	11.86	11.92	-0.06
Ethyl methacrylate	12.40	12.46	-0.06
Ethyl methyl carbonate	9.40	9.45	-0.05
Ethyl methyl disulfide	12.90	12.66	0.24
Ethyl methyl ketone oxime	9.88	9.90	-0.02
Ethyl methyl sulfide	9.45	9.41	0.04
Ethyl myristate	31.01	30.91	0.10
Ethyl N,N-diethylamino phosphorusoxy chloride	18.33	18.32	0.01
Ethyl N-butylcarbamate	15.69	15.68	0.01
Ethyl nicotinate	15.99	15.87	0.12
Ethyl nitroacetate	11.29	11.16	0.13
Ethyl N-methylcarbamate	10.19	10.19	0.00
Ethyl nonanoate	21.68	21.73	-0.05
Ethyl N-phenylcarbamate	18.50	18.48	0.02
Ethyl N-phenylformimide	18.12	17.78	0.34
Ethyl oleate	38.05	38.17	-0.12
Ethyl orthoformate	15.71	15.71	0.00
Ethyl pentanoate	14.64	14.39	0.25
Ethyl pentyl carbonate	16.78	16.80	-0.02
Ethyl phenoxyacetate	19.43	19.31	0.12
Ethyl phenyl butoxyborine	24.22	24.20	0.02
Ethyl phenyl fluorophosphate	18.23	18.31	-0.08
Ethyl phenylacetate	18.46	18.62	-0.16
Ethyl phenylglyoxylate	19.10	18.73	0.37
Ethyl pivalate	14.31	14.38	-0.07
Ethyl propanoate	10.70	10.72	-0.02
Ethyl propiolate	10.00	9.91	0.09
Ethyl propyl carbonate	13.09	13.13	-0.04
Ethyl propyl fluorophosphate	14.13	14.23	-0.10
Ethyl propyl sulfide	13.16	13.16	0.00
Ethyl pyruvate	10.65	10.83	-0.18
Ethyl ricinoleate	38.75	38.73	0.02
Ethyl salicylate	17.95	17.49	0.46
Ethyl t-butyl ether	12.62	12.51	0.11
Ethyl t-butyl ketone	13.70	13.79	-0.09
Ethyl thiocyanate	9.54	9.47	0.07
Ethyl trans-2-methyl-2-butenolate	14.38	14.34	0.04
Ethyl tribromoacetate	18.22	18.37	-0.15
Ethyl trichloroacetate	14.75	14.72	0.03
Ethyl trifluoroacetate	9.04	8.99	0.05
Ethyl tris(2,2-diethylhydrazino)silane	38.42	38.38	0.04

Ethyl undecanoate	25.35	25.40	-0.05
Ethyl vinyl ether	8.66	8.58	0.08
Ethylacetamide	9.55	9.53	0.02
Ethylamine	5.92	5.88	0.04
Ethylaminotriethylsilane	20.40	20.36	0.04
Ethylammonium nitrate	9.57	9.56	0.01
Ethylbenzene	14.25	14.25	0.00
Ethylbenzene sulfonate	18.09	18.12	-0.03
Ethylcyclobutane	11.15	11.00	0.15
Ethylcyclohexane	14.67	14.67	0.00
Ethylcyclohexyldifluorosilane	17.56	17.54	0.02
Ethylcyclopentane	12.84	12.83	0.01
Ethylcyclopropane	9.45	9.16	0.29
Ethyl dibutoxysilane	23.64	23.69	-0.05
Ethyl diisopropylamin	17.25	16.99	0.26
Ethyl dimethyl 1-(3-pentoxo)ethoxysilane	25.72	25.74	-0.02
Ethyl dimethylamine	9.73	9.74	-0.01
Ethylene glycol diformate	9.69	9.68	0.01
Ethylene glycol dimethacrylate	20.18	20.40	-0.22
Ethylene glycol monostearate	38.40	38.81	-0.41
Ethylene glycol monosulfite	7.94	8.15	-0.21
Ethylenediamine	7.22	7.24	-0.02
Ethylenedichloride	8.34	8.32	0.02
Ethylepoxide	8.07	8.02	0.05
Ethylidenecyclohexane	14.60	14.63	-0.03
Ethyl iodoacetylene	12.57	12.44	0.13
Ethyl-isoamylketone	15.52	15.62	-0.10
Ethylisobutylsilanol	16.01	16.04	-0.03
Ethylisopropylether	10.97	10.70	0.27
Ethylisopropylketone	11.76	11.95	-0.19
Ethylmethylether	6.93	7.01	-0.08
Ethyl-n-hexylether	16.24	16.20	0.04
Ethyl nitrate	7.63	7.54	0.09
Ethyl nitrite	6.97	6.94	0.03
Ethyl-n-propylether	10.69	10.69	0.00
Ethylphenylboronic acid	16.70	16.47	0.23
Ethylphenylboronic anhydride	32.73	32.42	0.31
Ethylphenylchlorosilane	19.60	19.82	-0.22
Ethylphenylphosphinic chloride	17.98	17.85	0.13
Ethyl-phenyl-propylthiophosphine	27.21	26.99	0.22
Ethylphosphinic dichloride	12.02	12.13	-0.11
Ethylphosphonyl difluoride	7.60	7.56	0.04

Ethylpropylphosphinic chloride	13.79	13.83	-0.04
Ethylsulfinyl chloride	10.27	10.21	0.06
Ethylthio dioctyl borane	38.86	39.05	-0.19
Ethylthiodiethylborane	16.97	17.02	-0.05
Ethyltributoxysilane	31.18	31.30	-0.12
Ethyltrichlorosilane	13.41	13.48	-0.07
Ethyltriethoxysilane	20.41	20.28	0.13
Ethyltriisothiocyanatosilane	25.44	25.56	-0.12
Ethyltrimethoxysilane	14.67	14.74	-0.07
Ethyne	3.33	3.50	-0.17
Ethynylbenzene	13.81	13.45	0.36
Etohexadiol	16.70	16.64	0.06
Eucarvone	18.73	18.32	0.41
Exalgin	17.93	17.84	0.09
Exaltol	28.05	28.09	-0.04
exo-Dicyclopentadiene	16.71	16.43	0.28
Farnesol	28.58	28.78	-0.20
Fenchlorphos	27.49	27.61	-0.12
Fenchone	17.74	17.58	0.16
Fichtelite	32.91	33.07	-0.16
Fluorene	21.68	21.45	0.23
Fluoro-2,4,6-trimethylbenzene	15.99	16.19	-0.20
Fluoroacetone	6.63	6.43	0.20
Fluorobenzene	10.37	10.47	-0.10
Fluoroethane	4.43	4.49	-0.06
Fluoroethyldiisopropylsilane	18.91	18.98	-0.07
Fluorotributylsilane	26.44	26.28	0.16
Fluorotriethylsilane	15.10	15.27	-0.17
Fluorotripentylsilane	31.83	31.78	0.05
Fluorotripropylsilane	20.74	20.77	-0.03
Formaldehyde diethylacetal	11.36	11.28	0.08
Formamide	4.21	3.99	0.22
Formanilide	14.29	14.22	0.07
Formic acid	3.39	3.37	0.02
Freon 113	10.37	10.33	0.04
Fulvene	10.90	10.76	0.14
Fumaric acid dichloride	12.67	12.44	0.23
Furan	7.20	7.54	-0.34
Furfural	10.08	9.62	0.46
Furfuranol	9.90	9.97	-0.07
Furfuryl butyrate	17.33	17.45	-0.12
Furfuryl propionate	15.42	15.61	-0.19

Furfurylacetate	13.72	13.78	-0.06
gamma-Butyrolactone	7.90	8.04	-0.14
gamma-Caprolactone	11.84	11.71	0.13
gamma-Coniceine	15.71	15.94	-0.23
gamma-Octanoic lactone	15.32	15.38	-0.06
gamma-Terpinene	17.96	18.23	-0.27
gamma-Undecanolactone	20.72	20.89	-0.17
gamma-Valerolactone	9.77	9.87	-0.10
Geranyl 2-methylpropanoate	26.95	27.12	-0.17
Geranyl acetate	23.36	23.46	-0.10
Glutaconodinitrile	9.92	9.78	0.14
Glycerol 1,3-dinitrate	13.26	12.96	0.30
Glycerol 1-butanoate	15.40	15.51	-0.11
Glycerol 1-oleate	41.29	41.13	0.16
Glycerol tricaproate	41.14	41.48	-0.34
Glycerol tristearate	107.48	107.55	-0.07
Glyceryl tributanoate	30.27	30.46	-0.19
Glyceryl-1-nitrate	10.70	10.50	0.20
Glyceryltriacetate	19.30	19.45	-0.15
Glycidyl acrylate	12.26	12.26	0.00
Glycidyl methacrylate	14.48	14.12	0.36
Glycolaldehyde	4.93	5.28	-0.35
Glyme	9.51	9.51	0.00
Glyoxal	4.70	4.93	-0.23
Guaiol	27.18	27.15	0.03
Hemimellitene	16.03	16.23	-0.20
Heneicosane	39.44	39.39	0.05
Heptacosane	50.47	50.40	0.07
Heptadecane	32.09	32.05	0.04
Heptadecanonitrile	32.01	31.97	0.04
Heptadecylbenzene	41.79	41.78	0.01
Heptafluorobutanoic anhydride	17.41	17.07	0.34
Heptafluorobutanoyl chloride	10.71	10.77	-0.06
Heptaldoxime	15.13	15.48	-0.35
Heptane	13.72	13.70	0.02
Heptanedioic acid	14.90	14.96	-0.06
Heptanoamide	15.27	14.94	0.33
Heptanoic anhydride	26.82	27.25	-0.43
Heptanonitrile	13.48	13.61	-0.13
Heptanophenone	23.55	23.54	0.01
Heptanoyl chloride	16.01	15.86	0.15
Heptasilane	33.60	33.63	-0.03



Heptyl 1-naphthaleneacetate	34.77	34.91	-0.14
Heptyl 1-naphthoate	33.29	33.08	0.21
Heptyl 1-naphthylketone	32.56	32.49	0.07
Heptyl 2-naphthaleneacetate	34.89	34.91	-0.02
Heptyl 2-thiophenecarboxylate	25.58	25.35	0.23
Heptyl bromide	16.74	16.76	-0.02
Heptyl butyrate	21.78	21.73	0.05
Heptyl pentanoate	23.57	23.57	0.00
Heptylbenzene	23.44	23.43	0.01
Heptylcyclohexane	23.88	23.84	0.04
Heptylcyclopentane	22.04	22.01	0.03
Heptyliodoacetylene	21.61	21.61	0.00
Heptyloxytrimethylsilane	23.31	23.32	-0.01
Heptylphosphinic dichloride	21.24	21.30	-0.06
Hexabromoethane	23.58	23.49	0.09
Hexachloroacetone	18.04	18.13	-0.09
Hexachlorobutadiene	19.75	19.62	0.13
Hexachloropropylene	17.77	17.91	-0.14
Hexacosane	48.80	48.57	0.23
Hexacosanoic acid	49.56	49.20	0.36
Hexadecamethylheptasiloxane	56.41	56.37	0.04
Hexadecanedioic acid	31.43	31.48	-0.05
Hexadecanenitrile	30.17	30.13	0.04
Hexadecanoyl chloride	32.56	32.38	0.18
Hexadecyl acetate	34.92	34.58	0.34
Hexadecyl vinyl ether	34.46	34.28	0.18
Hexadecylamine	31.62	31.57	0.05
Hexadecylbenzene	39.95	39.95	0.00
Hexadecylcyclohexane	40.65	40.36	0.29
Hexaethyl tetraphosphate	39.91	39.92	-0.01
Hexaethylbenzene	33.03	32.96	0.07
Hexaethyldisiloxane	30.09	30.27	-0.18
Hexaethylene glycol	27.22	27.34	-0.12
Hexaethyltetraphosphate	39.91	39.92	-0.01
Hexafluorobenzene	10.50	10.27	0.23
Hexafluoropropyl-1,3-diisocyanate	12.36	12.22	0.14
Hexahydro-1-methyl-1H-1,4-diazepine	14.04	13.88	0.16
Hexamethyldisilane	20.38	20.36	0.02
Hexamethyldisiloxane	19.40	19.40	0.00
Hexane	11.80	11.86	-0.06
Hexanenitrile	11.77	11.78	-0.01
Hexanoic anhydride	23.74	23.58	0.16

Hexanophenone	21.56	21.70	-0.14
Hexanoyl chloride	13.98	14.02	-0.04
Hexapropyldisiloxane	41.25	41.29	-0.04
Hexasilane	28.85	28.86	-0.01
Hexyl 1-naphthaleneacetate	32.88	33.08	-0.20
Hexyl 1-naphthoate	31.44	31.24	0.20
Hexyl 1-naphthylketone	30.69	30.66	0.03
Hexyl 2-naphthaleneacetate	33.10	33.08	0.02
Hexyl 2-naphthoate	31.66	31.24	0.42
Hexyl 2-thiophenecarboxylate	23.72	23.52	0.20
Hexyl bromide	14.91	14.93	-0.02
Hexyl butanoate	19.81	19.90	-0.09
Hexyl cyclohexyloxy dithiophosphinic acid	32.28	32.36	-0.08
Hexyl dichloro phosphorus thioxide	22.39	22.38	0.01
Hexyl hexanoate	23.54	23.57	-0.03
Hexyl hexyloxy dithiophosphinic acid	33.21	33.20	0.01
Hexyl isopentoxy dithiophosphinic acid	31.37	31.35	0.02
Hexyl methacrylate	19.77	19.80	-0.03
Hexyl methoxy dithiophosphinic acid	23.94	24.01	-0.07
Hexyl nitrite	14.31	14.28	0.03
Hexyl octanoate	27.31	27.24	0.07
Hexyl octyloxy dithiophosphinic acid	36.79	36.87	-0.08
Hexyl pentanoate	21.77	21.73	0.04
Hexyl perfluorobutyrate	20.40	20.31	0.09
Hexyl phenyl sulfide	24.96	24.89	0.07
Hexyl propanoate	18.48	18.06	0.42
Hexylbenzene	21.55	21.60	-0.05
Hexylcyclohexane	22.04	22.01	0.03
Hexylcyclopentane	20.20	20.17	0.03
Hexyldichloroborane	17.47	17.45	0.02
Hexyleneglycol	13.05	12.96	0.09
Hexyloxybenzene	22.35	22.29	0.06
Hexyloxytrimethylsilane	21.47	21.48	-0.01
Hexylphosphinic dichloride	19.77	19.47	0.30
Hexylsilane	15.99	15.97	0.02
HMDS	20.43	20.34	0.09
Homocamfin	18.57	18.38	0.19
Hydroabietyl acrylate	40.60	40.96	-0.36
Hydrocinnamitrile	15.95	16.01	-0.06
Hydrocinnamyl alcohol	16.91	16.65	0.26
Hydroxycitronellal	19.88	19.93	-0.05
Imidazole	7.44	7.39	0.05

Indane	15.20	15.31	-0.11
Indene	15.32	15.23	0.09
Iodoacetonitrile	9.47	9.54	-0.07
Iodobenzene	15.52	15.50	0.02
Iodocyclopentane	14.37	14.41	-0.04
Iodopentafluorobenzene	15.36	15.30	0.06
Iodopentafluoroethane	9.78	9.71	0.07
Iophendylate	40.46	40.10	0.36
Isoamyl acetate	14.43	14.37	0.06
iso-Amyl dichloro phosphorus oxide	17.05	17.24	-0.19
iso-Amyl dichloro phosphorus thioxide	20.54	20.53	0.01
Isoamyl iodide	15.11	15.11	0.00
Isoamyl lactate	16.72	16.77	-0.05
Isoamylisonitrile	11.74	11.96	-0.22
Isobutyric anhydride	16.16	16.21	-0.05
Isobutyl 2-chloropropionate	16.17	16.26	-0.09
Isobutyl 3-chloropropionate	16.32	16.28	0.04
Isobutyl acetate	12.53	12.54	-0.01
Isobutyl acrylate	14.30	14.25	0.05
Isobutyl allyloxy dithiophosphinic acid	23.74	23.93	-0.19
Isobutyl bromide	11.14	11.24	-0.10
Isobutyl butyrate	16.69	16.21	0.48
Isobutyl chloride	10.10	10.08	0.02
Isobutyl chlorocarbonate	12.78	12.69	0.09
Isobutyl cyclohexylchloroboronate	22.58	22.50	0.08
Isobutyl dichloro phosphorus oxide	15.45	15.45	0.00
Isobutyl diisobutoxy phosphorus	27.60	27.38	0.22
Isobutyl ethoxyethoxy dithiophosphinic acid	26.52	26.56	-0.04
Isobutyl ethoxyethoxy S-(2-cyanoethyl) dithiophosphinate	31.70	31.82	-0.12
Isobutyl formate	10.83	10.75	0.08
Isobutyl iodide	13.29	13.28	0.01
Isobutyl isobutyrate	16.22	16.19	0.03
Isobutyl isopropoxy dithiophosphinic acid	24.15	24.06	0.09
Isobutyl isopropoxy S-methoxycarbonylethyl dithiophosphinate	32.16	31.92	0.24
Isobutyl isothiocyanate	13.96	13.98	-0.02
Isobutyl isovalerate	18.05	18.03	0.02
Isobutyl methacrylate	16.10	16.11	-0.01
Isobutyl methyl ketone	11.98	11.95	0.03
Isobutyl nitrate	11.34	11.19	0.15
Isobutyl propanoate	14.00	14.37	-0.37

Isobutyl ricinoleate	42.15	42.39	-0.24
Isobutyl salicylate	21.60	21.14	0.46
Isobutyl t-butylether	16.32	16.17	0.15
Isobutyl trichloroacetate	18.44	18.37	0.07
Isobutyl urethane	15.73	15.67	0.06
Isobutyl valerate	17.81	18.04	-0.23
Isobutyl vinyl ether	12.48	12.24	0.24
Isobutylbenzene	17.92	17.91	0.01
Isobutylcyclohexane	18.38	18.32	0.06
Isobutylcyclopentane	16.63	16.49	0.14
Isobutyldimethylamine	13.42	13.39	0.03
Isobutylnitrite	10.67	10.59	0.08
iso-Butylsilane	12.31	12.29	0.02
Isobutyronitrile	8.08	8.09	-0.01
Isobutyroylbromide	11.55	11.51	0.04
Isobutyroylchloride	10.24	10.34	-0.10
Isocrotonic acid	8.85	8.74	0.11
Isocumene	16.02	16.09	-0.07
Isodecyl acrylate	25.14	25.26	-0.12
Isofluorophate	16.14	16.07	0.07
Isohexanoic acid	12.48	12.48	0.00
Isooctane	15.46	15.51	-0.05
Isopentane	10.03	10.01	0.02
Isopentene	9.85	9.93	-0.08
Isopentyl 2-chloropropanoate	18.16	18.10	0.06
Isopentyl alcohol	10.58	10.57	0.01
Isopentyl bromide	13.12	13.08	0.04
Isopentyl butanoate	18.00	18.04	-0.04
Isopentyl chloride	11.92	11.91	0.01
Isopentyl dichloro phosphorus oxide	17.24	17.28	-0.04
Isopentyl ethoxyethoxy dithiophosphinic acid	28.39	28.39	0.00
Isopentyl formate	12.64	12.59	0.05
Isopentyl isopentanoate	19.84	19.86	-0.02
iso-Pentyl isopropoxy dithiophosphinic acid	25.96	25.85	0.11
Isopentyl methoxyethoxy dithiophosphinic acid	26.50	26.55	-0.05
Isopentyl nitrite	12.52	12.43	0.09
Isopentyl propionate	16.18	16.21	-0.03
Isopentyl propoxy dithiophosphinic acid	25.93	25.89	0.04
Isopentyl salicylate	23.36	22.98	0.38
Isopentylamine	11.36	11.37	-0.01
Isopentylbenzene	19.73	19.74	-0.01
Isopentyloxytrimethylsilane	19.64	19.63	0.01

Isophorol	17.02	17.02	0.00
Isophthaloylchloride	19.02	18.65	0.37
Isophytol	37.59	37.92	-0.33
Isoprene	10.10	9.81	0.29
Isopropanolamine	8.29	8.28	0.01
Isopropenyl methyl ketone	9.94	10.04	-0.10
Isopropenylacetate	10.66	10.48	0.18
Isopropenylacetylene	9.32	9.12	0.20
Isopropyl (2,4-dichlorophenoxy)acetate	25.20	24.97	0.23
Isopropyl 2-(2,3-dihydroxypropoxy)ethyl thioether	20.49	20.46	0.03
Isopropyl 2-chloropropanoate	14.49	14.46	0.03
Isopropyl 2-furoate	15.95	15.62	0.33
Isopropyl 3-methylbutanoate	16.09	16.21	-0.12
Isopropyl acetoacetate	14.62	14.50	0.12
Isopropyl benzoate	18.48	18.62	-0.14
Isopropyl butyrate	14.36	14.39	-0.03
Isopropyl chloroacetate	13.06	12.63	0.43
Isopropyl formate	9.00	8.94	0.06
Isopropyl hydroperoxide	7.94	7.84	0.10
Isopropyl isocyanate	9.08	9.13	-0.05
Isopropyl isopropanethiolsulfinate	18.83	18.89	-0.06
Isopropyl lactate	12.95	13.12	-0.17
Isopropyl laurate	28.96	29.08	-0.12
Isopropyl methacrylate	14.29	14.30	-0.01
Isopropyl methyl ether	8.91	8.85	0.06
Isopropyl methyl sulfide	11.34	11.24	0.10
Isopropyl myristate	32.62	32.75	-0.13
Isopropyl N,N-diethylamino phosphorusoxy chloride	20.14	20.18	-0.04
Isopropyl N,N-diethylamino phosphorusoxy fluoride	17.83	17.82	0.01
Isopropyl nicotinate	17.90	17.71	0.19
Isopropyl palmitate	36.85	36.42	0.43
Isopropyl pentanoate	16.37	16.23	0.14
Isopropyl propionate	12.52	12.56	-0.04
Isopropyl propyl ether	12.61	12.53	0.08
Isopropyl salicylate	19.80	19.32	0.48
Isopropyl trichloroacetate	16.72	16.56	0.16
Isopropyl trifluoroacetate	11.29	10.83	0.46
Isopropyl vinyl ether	10.60	10.42	0.18
Isopropylacetate	10.69	10.72	-0.03
Isopropylamine	7.77	7.69	0.08
Isopropylcyclohexane	16.47	16.49	-0.02
Isopropylcyclopentane	14.67	14.65	0.02

Isopropylcyclopropane	11.31	10.98	0.33
Isopropylisopropoxyphosphinic chloride	16.10	16.07	0.03
Isopropylmethylsilane	12.15	12.24	-0.09
Isopropylnitrate	9.58	9.38	0.20
Isopropylphenylether	16.81	16.78	0.03
Isopropylphenylphosphinic chloride	20.09	19.71	0.38
Isopropylphosphonyl difluoride	9.34	9.42	-0.08
Isopropylpropoxyphosphinic chloride	16.12	16.06	0.06
Isopropylsulfinyl chloride	11.82	12.04	-0.22
Isopropylsulfonic acid	10.78	10.56	0.22
Isopropylsulfonyl fluoride	10.21	10.16	0.05
Isopropylthioacetate	13.09	13.30	-0.21
Isopropyltriisothiocyantosilane	27.56	27.41	0.15
Isopropyltrimethylsilane	15.25	15.69	-0.44
Isopulegol	18.81	18.79	0.02
Isopulegol acetate	22.89	22.59	0.30
Isoquinaldine	18.25	18.69	-0.44
Isoquinoline	16.38	16.72	-0.34
Isovaleraldehyde	10.15	10.22	-0.07
Isovaleronitrile	9.93	9.93	0.00
Isoxazole	6.56	6.66	-0.10
Jasmone	20.22	20.19	0.03
Ketene	4.40	4.49	-0.09
Lactonitrile	7.00	6.83	0.17
L-Alanine 1-methylethyl ester dodecyl sulfate	40.78	40.95	-0.17
L-Alanine 2-methylpropyl ester dodecyl sulfate	42.57	42.76	-0.19
Lauric acid	23.07	23.51	-0.44
Laurocapram	34.22	34.53	-0.31
Lauronitrile	22.81	22.79	0.02
Linalool	19.35	19.57	-0.22
Linalyl acetate	23.19	23.37	-0.18
Linoleic acid	34.37	34.36	0.01
L-Menthone	18.37	18.41	-0.04
Longifolene	25.74	25.67	0.07
L-Proline 1-methylethyl ester dodecyl sulfate	43.73	43.83	-0.10
Lupeol	51.80	52.02	-0.22
L-Valine 1-methylethyl ester dodecyl sulfate	44.65	44.60	0.05
m-Anisidine	14.81	14.71	0.10
Margaric acid	32.73	32.68	0.05
m-Cresol	13.01	13.12	-0.11
m-Cresylacetate	16.72	16.87	-0.15
Mecrylate	10.60	10.53	0.07

Menthol	18.79	18.87	-0.08
Menthone	18.36	18.41	-0.05
Menthyl isovalerate	28.13	28.16	-0.03
Menthylacetate	22.86	22.67	0.19
Mercaptoacetic acid	8.21	8.19	0.02
Mesoxalic acid diethylester oxime	17.19	16.79	0.40
Metasystox	22.61	22.77	-0.16
Methacrolein	8.27	8.30	-0.03
Methacryloyl chloride	10.12	10.26	-0.14
Methanesulfonic acid	6.67	6.81	-0.14
Methanesulfonylchloride	8.36	8.09	0.27
Methanol	3.26	3.23	0.03
Metharbital	18.81	19.07	-0.26
Methoxy(methoxymethoxy)methane	10.15	10.00	0.15
Methoxyacetaldehyde	7.00	7.22	-0.22
Methoxyacetic acid	7.63	7.65	-0.02
Methoxyacetonitrile	6.93	6.93	0.00
Methoxyacetyl chloride	9.17	9.18	-0.01
Methoxyacetylene	6.43	6.24	0.19
Methoxydichloromethylsulfenyl chloride	14.32	14.33	-0.01
Methoxytriethylsilane	17.64	17.73	-0.09
Methoxytrimethylsilane	12.21	12.29	-0.08
Methoxytripropylsilane	23.24	23.23	0.01
Methyl (Z) 9-octadecenoate	36.29	36.32	-0.03
Methyl 10-undecenoate	23.27	23.43	-0.16
Methyl 1-naphthoate	21.97	22.06	-0.09
Methyl 1-naphthylacetate	23.69	23.89	-0.20
Methyl 2,3-dibromopropanoate	15.15	15.03	0.12
Methyl 2-benzoylbenzoate	27.04	26.69	0.35
Methyl 2-chloroacrylate	10.63	10.70	-0.07
Methyl 2-furoate	12.18	11.93	0.25
Methyl 2-hydroxy-3-methylbenzoate	17.56	17.54	0.02
Methyl 2-hydroxy-5-methylbenzoate	17.57	17.54	0.03
Methyl 2-methoxybenzoate	17.70	17.52	0.18
Methyl 2-methylacetoacetate	12.67	12.63	0.04
Methyl 2-naphthaleneacetate	23.79	23.89	-0.10
Methyl 2-octynoate	17.62	17.45	0.17
Methyl 2-thiophenecarboxylate	14.44	14.33	0.11
Methyl 3-(methylthio)propanoate	13.66	13.76	-0.10
Methyl 3,3-dimethylacrylate	12.57	12.49	0.08
Methyl 3-butenolate	10.43	10.58	-0.15
Methyl 3-chlorobutyrate	12.31	12.59	-0.28

Methyl 3-cyclohexene-1-carboxylate	15.05	15.27	-0.22
Methyl 3-hexenoate	14.20	14.30	-0.10
Methyl 3-mercaptopropanoate	12.11	11.91	0.20
Methyl 3-methoxybenzoate	17.77	17.52	0.25
Methyl 3-methoxypropanoate	11.27	11.36	-0.09
Methyl 3-methylbutyrate	12.47	12.53	-0.06
Methyl 4-bromo-2-butenate	13.96	13.70	0.26
Methyl 4-bromobutanoate	13.95	13.77	0.18
Methyl 4-chlorobutyrate	12.44	12.61	-0.17
Methyl 4-chlorophenylphosphinic chloride	18.08	17.98	0.10
Methyl 5-bromovalerate	15.63	15.61	0.02
Methyl abietate	37.20	37.36	-0.16
Methyl acetate	6.96	7.04	-0.08
Methyl acrylate	8.75	8.75	0.00
Methyl benzenesulfonate	16.17	16.28	-0.11
Methyl benzoate	15.05	14.94	0.11
Methyl benzoylacetate	19.05	18.71	0.34
Methyl bis(2,2-diethylhydrazino)silane	26.63	26.69	-0.06
Methyl bis(2,2-dimethylhydrazino)silane	19.34	19.41	-0.07
Methyl bis(2-chloropropoxy)silane	21.95	21.98	-0.03
Methyl bis(diethylamino)silane	23.78	23.67	0.11
Methyl bromoacetate	10.01	10.10	-0.09
Methyl but-3-yne-1-carboxylate	11.62	11.73	-0.11
Methyl carbamate	6.52	6.40	0.12
Methyl cellosolve	7.66	7.57	0.09
Methyl chlorocarbonate	7.21	7.19	0.02
Methyl chlorofluorophosphate	8.21	8.21	0.00
Methyl chlorooxoacetate	9.21	9.20	0.01
Methyl crotonate	10.73	10.63	0.10
Methyl cyclobutanecarboxylate	11.78	11.68	0.10
Methyl cyclohexanecarboxylate	15.02	15.35	-0.33
Methyl cyclopropanecarboxylate	10.08	9.84	0.24
Methyl decanoate	21.67	21.72	-0.05
Methyl dichloroacetate	10.90	10.87	0.03
Methyl dimethylmalonate	14.96	15.05	-0.09
Methyl formate	5.17	5.25	-0.08
Methyl hexanoate	14.29	14.38	-0.09
Methyl hydrocinnamate	18.44	18.61	-0.17
Methyl isoamyl ketone	13.66	13.79	-0.13
Methyl isobutanoate	10.63	10.69	-0.06
Methyl isonicotinate	14.10	14.02	0.08
Methyl laurate	25.32	25.39	-0.07



Methyl levulinate	12.51	12.65	-0.14
Methyl linolenate	36.20	36.16	0.04
Methyl methacrylate	10.58	10.61	-0.03
Methyl methanesulfonate	8.42	8.20	0.22
Methyl methanethiosulfinate	11.41	11.39	0.02
Methyl methoxyacetate	9.44	9.53	-0.09
Methyl N,N-diethylamino phosphorusoxy chloride	16.48	16.53	-0.05
Methyl N,N-diethylamino phosphorusoxy fluoride	14.29	14.17	0.12
Methyl nonanoate	19.70	19.88	-0.18
Methyl octadecanoate	36.46	36.40	0.06
Methyl octanoate	17.98	18.05	-0.07
Methyl pentadecanoate	30.88	30.90	-0.02
Methyl pentafluoropropanoate	9.11	9.13	-0.02
Methyl pentyl sulfide	14.96	14.92	0.04
Methyl perfluorobutanoate	11.23	11.12	0.11
Methyl perfluorooctanoate	19.07	19.06	0.01
Methyl phenoxyacetate	17.30	17.46	-0.16
Methyl phenylacetate	16.69	16.77	-0.08
Methyl pivalate	12.26	12.53	-0.27
Methyl propanoate	8.79	8.87	-0.08
Methyl propenyl ketone	10.09	10.05	0.04
Methyl propyl disulfide	14.74	14.50	0.24
Methyl propyl sulfide	11.28	11.25	0.03
Methyl pyruvate	8.59	8.98	-0.39
Methyl t-butyl disulfide	16.43	16.48	-0.05
Methyl tert-pentyl sulfide	15.20	14.91	0.29
Methyl tetradecanoate	29.04	29.06	-0.02
Methyl tiglate	12.68	12.49	0.19
Methyl t-pentyl ether	12.43	12.50	-0.07
Methyl trichloroacetate	12.88	12.87	0.01
Methyl trichloromethyl ether	11.13	10.92	0.21
Methyl tridecanoate	27.22	27.22	0.00
Methyl trifluoroacetate	7.19	7.15	0.04
Methyl tris(2,2-diethylhydrazino)silane	36.57	36.56	0.01
Methyl undecanoate	23.50	23.55	-0.05
Methyl valerate	12.49	12.54	-0.05
Methyl vinyl ether	6.79	6.73	0.06
Methyl Z,Z-9,12-octadecadieneoate	36.23	36.24	-0.01
Methyl-1chloroethylether	9.18	8.96	0.22
Methylacetamide	7.82	7.71	0.11
Methylacetoacetate	10.79	10.81	-0.02
Methylamine	4.01	4.06	-0.05

Methylbenzene	12.31	12.42	-0.11
Methylbutylphosphinic chloride	13.88	13.88	0.00
Methylchloroacetate	8.84	8.94	-0.10
Methylchloroform	10.37	10.35	0.02
Methylconiine	18.21	18.02	0.19
Methylcyanoacetate	8.81	8.79	0.02
Methylcyclobutane	9.50	9.16	0.34
Methylcyclohexane	12.88	12.83	0.05
Methylcyclohexyldifluorosilane	15.73	15.73	0.00
Methylcyclohexylether	13.50	13.51	-0.01
Methylcyclopentane	11.04	11.00	0.04
Methylcyclopropylketone	9.49	9.27	0.22
Methyldibutoxysilane	21.75	21.88	-0.13
Methyldichloro-2-(2,4-dichlorophenoxy)ethylsilane	27.87	27.80	0.07
Methyldichloro-2-(4-chlorophenoxy)ethylsilane	25.96	25.88	0.08
Methyldichloro-2,4-dichlorophenoxysilane	24.16	23.86	0.30
Methyldichloro-2-butoxyethylsilane	21.85	21.56	0.29
Methyldichloro-2-isobutoxyethylsilane	21.61	21.54	0.07
Methyldichloro-2-phenoxyethylsilane	23.94	23.97	-0.03
Methyldichloro-4-chlorophenoxysilane	21.83	21.95	-0.12
Methyldichlorobutoxysilane	17.70	17.70	0.00
Methyldichlorophenoxysilane	19.88	20.04	-0.16
Methyldiethyl-2-phenoxyethylsilane	27.78	27.88	-0.10
Methyldiethylphenoxysilane	23.90	23.78	0.12
Methylelaidate	36.27	36.32	-0.05
Methylenanthate	16.25	16.21	0.04
Methylenebis(4-cyclohexylisocyanate)	28.55	28.54	0.01
Methylenecyclobutane	9.25	9.08	0.17
Methylenecyclohexane	12.74	12.75	-0.01
Methylenecyclopentane	10.92	10.92	0.00
Methylethylphosphinic chloride	10.29	10.21	0.08
Methylhydroperoxide	4.26	4.15	0.11
Methylisobutylphosphinic chloride	13.92	13.87	0.05
Methylisocyanate	5.16	5.51	-0.35
Methylisopropylphosphinic chloride	11.84	12.07	-0.23
Methylisothiocyanate	8.32	8.50	-0.18
Methylactate	9.44	9.43	0.01
Methylnitrate	5.79	5.69	0.10
Methylnonylphenylsilane	32.86	32.71	0.15
Methyl-n-pentylether	12.54	12.52	0.02
Methyl-n-propylketone	9.99	10.13	-0.14
Methyloctylphenylsilane	30.99	30.88	0.11

Methyloxiran	6.01	6.18	-0.17
Methylphenyldifluorosilane	15.17	15.29	-0.12
Methylphenylphosphinic chloride	15.91	16.07	-0.16
Methylphenylsilane	16.18	16.46	-0.28
Methylphosphonic acid dimethyl ester	10.43	10.56	-0.13
Methylphosphonyl difluoride	5.81	5.77	0.04
Methylphosphoric acid ethylester	10.68	10.40	0.28
Methylpropylether	8.77	8.85	-0.08
Methylpropylphosphinic chloride	12.04	12.05	-0.01
Methylpropylsilane	12.18	12.22	-0.04
Methylsalicylate	15.90	15.64	0.26
Methylsilanetriol triacetate	18.34	18.34	0.00
Methylsulfinyl chloride	8.44	8.29	0.15
Methylsulfonyl fluoride	6.32	6.41	-0.09
Methylthiirane	8.74	8.64	0.10
Methylthiocyanate	7.53	7.56	-0.03
Methyltri(2-octyloxy)silane	51.47	51.52	-0.05
Methyltributoxysilane	29.49	29.48	0.01
Methyltrichlorosilane	11.55	11.67	-0.12
Methyltriheptyloxysilane	45.99	46.00	-0.01
Methyltrihexyloxysilane	40.48	40.50	-0.02
Methyltriisopentyloxysilane	34.99	34.94	0.05
Methyltripentyloxysilane	34.96	34.99	-0.03
Methyltriphenoxysilane	36.41	36.52	-0.11
Methylvinylchlorosilane	13.21	13.40	-0.19
Monoamyl adipate	22.46	22.36	0.10
Monobutyl adipate	20.57	20.53	0.04
Monobutyl succinate	16.82	16.86	-0.04
Monoethyl adipate	16.86	16.86	0.00
Monohexyl adipate	24.44	24.20	0.24
Monomethyl adipate	14.95	15.01	-0.06
Monomethyl glutarate	13.01	13.18	-0.17
Monopropyl adipate	18.69	18.69	0.00
Montanic acid	53.24	52.87	0.37
Morpholine	9.36	9.35	0.01
Morpholinium formate	12.76	12.79	-0.03
MTBE	10.58	10.66	-0.08
m-Toluidine	14.05	14.03	0.02
Muscone	29.13	29.46	-0.33
Mustard gas	15.32	15.13	0.19
Mustard oil	12.00	12.03	-0.03
Myrcene	18.88	18.93	-0.05

Myristicin	20.95	20.97	-0.02
Myristonitrile	26.37	26.46	-0.09
N-(1,1-Dimethylpropyl)aminotriethylsilane	25.68	25.84	-0.16
N-(1-Naphthyl)ethylenediamine	24.61	24.37	0.24
N-(2',3'-Epoxypropyl)-N-methylpyrrolidonium acetate	22.00	21.59	0.41
N-(2-Aminoethyl)ethanolamine	11.53	11.44	0.09
N-(2-Hydroxyethyl)-2-furfurylamine	14.81	14.98	-0.17
N-(2-Hydroxypropyl)-2-furfurylamine	16.74	16.82	-0.08
N-(2-Pyridinylmethyl)-2-pyridinemethanamine	23.59	23.64	-0.05
N-(3-(Trimethoxysilyl)propyl)-1,2-ethanediamine	23.07	22.94	0.13
N-(3-Aminopropyl)-N-methyl-1,3-propanediamine	17.82	17.95	-0.13
N-(Hydroxyethyl)piperazine	14.46	14.42	0.04
N,N,N',N'-Tetraethyl-1,2-ethylenediamine	22.03	22.23	-0.20
N,N,N',N'-Tetramethyl-1,6-hexanediamine	22.15	22.29	-0.14
N,N-Bis(2-hydroxyethyl)butylamine	18.17	18.16	0.01
N,N-Bis(2-hydroxyethyl)ethylamine	14.44	14.49	-0.05
N,N'-Dibenzyl-1,2-ethanediamine	30.24	30.33	-0.09
N,N-Dibutylaminotriethylsilane	31.18	31.44	-0.26
N,N-Dibutylaniline	27.32	27.05	0.27
N,N-Dibutyl-difluoroacetamide	20.77	20.65	0.12
N,N'-Diethyl-1,2-ethanediamine	14.49	14.53	-0.04
N,N-Diethyl-1,3-propanediamine	16.65	16.57	0.08
N,N-Diethyl-1-naphthalenamine	26.54	26.83	-0.29
N,N-Diethyl-3-methylbutanamide	18.83	18.84	-0.01
N,N-Diethylaminotriethylsilane	24.18	24.10	0.08
N,N-Diethylaniline	19.97	19.71	0.26
N,N-Diethylbutanamide	16.85	17.02	-0.17
N,N-Diethylformamide	11.46	11.57	-0.11
N,N-Diethylhydroxylamine	10.30	10.27	0.03
N,N-Diethylpropanamide	15.12	15.19	-0.07
N,N'-Diethylurea	12.15	12.36	-0.21
N,N-Diisobutylaminotriethylsilane	31.18	31.41	-0.23
N,N-Dimethyl-1,2-ethanediamine	11.15	11.10	0.05
N,N-Dimethyl-1-naphthylamine	23.00	23.19	-0.19
N,N-Dimethyl-3-toluidine	18.12	17.98	0.14
N,N-Dimethylacrylamide	11.46	11.42	0.04
N,N-Dimethylaniline	16.21	16.07	0.14
N,N-Dimethylbenzylamine	17.66	17.64	0.02
N,N-Dimethylbutyramide	13.25	13.38	-0.13
N,N-Dimethylcyclohexylamine	16.09	16.20	-0.11
N,N-Dimethylethanolamine	10.29	10.29	0.00

N,N-Dimethylformamide	7.93	7.93	0.00
N,N-Dimethyl-N'-benzyl-1,2-ethanediamine	22.58	22.64	-0.06
N,N-Dimethylpentanamide	15.12	15.22	-0.10
N,N-Dimethylpropionamide	11.46	11.55	-0.09
N,N-Dimethyl-p-toluidine	17.86	17.98	-0.12
N,N-Dipropylaniline	23.74	23.38	0.36
N-Acetyethanolamine	10.25	10.09	0.16
N-Acetyl-N-methylacetamide	11.51	11.48	0.03
N-Allylaniline	17.61	17.60	0.01
n-Amyl ether	19.93	19.87	0.06
N-Benzyl-2-methylaniline	25.88	25.70	0.18
N-Benzyl-N-ethylhydroxylamine	18.14	18.17	-0.03
n-Butyl acetate	12.48	12.55	-0.07
n-Butyl acrylate	14.41	14.27	0.14
n-Butyl methyl ether	10.79	10.68	0.11
n-Butyl-2-chloropropanoate	16.32	16.28	0.04
n-Butyl-3-chloropropanoate	16.33	16.29	0.04
N-Butyl-3-methylpyridinium bis(trifluoromethylsulfonyl)amide	31.91	32.13	-0.22
N-Butyl-3-methylpyridinium trifluoromethanesulfonate	25.47	25.47	0.00
N-Butyl-4-methylthiazolium bis(trifluoromethylsulfonyl) amide	31.19	31.41	-0.22
N-Butyl-4-methylthiazolium difluoro(oxalato)borate	25.07	25.10	-0.03
N-Butylaniline	19.73	19.56	0.17
n-Butylbenzoate	20.57	20.45	0.12
n-Butylchloroacetate	14.40	14.46	-0.06
n-Butyldichloroacetate	16.42	16.38	0.04
N-Butyl-difluoroacetamide	13.50	13.16	0.34
n-Butylethylether	12.57	12.53	0.04
n-Butylformate	10.68	10.77	-0.09
n-Butylmethacrylate	16.10	16.13	-0.03
n-Butylmethylsulfide	13.12	13.08	0.04
n-Butylnitrite	10.64	10.61	0.03
N-Butyl-N-methylmorpholinium N-acetylalaninate	29.46	29.58	-0.12
N-Butyl-N-methylmorpholinium N-acetylleucinate	35.05	35.07	-0.02
N-Butyl-N-methylmorpholinium N-acetylvalinate	33.29	33.24	0.05
n-Butylnonanoate	25.56	25.40	0.16
N-Butyl-N-phenylacetamide	23.05	23.33	-0.28
N-Butylpiperidine	18.14	18.03	0.11
N-Butylpyridinium bis(trifluoromethanesulfonyl) amide	30.21	30.23	-0.02

N-Butylpyridinium triflate	23.49	23.56	-0.07
N-Butylpyridinium trifluoroacetate	21.75	21.96	-0.21
N-Butylthiazolium bis(trifluoromethylsulfonyl) amide	29.29	29.58	-0.29
N-Butylthiazolium difluoro(oxalato)borate	23.16	23.27	-0.11
n-Butyltrichloroacetate	18.39	18.39	0.00
n-Crotylacetate	12.41	12.47	-0.06
N-Cyclohexylaniline	22.15	22.36	-0.21
n-Decanoic acid	19.87	19.84	0.03
n-Decyl alcohol	19.82	19.76	0.06
n-Decylacetate	23.53	23.57	-0.04
n-Decylamine	20.58	20.56	0.02
N-Decylpyridinium bis(trifluoromethanesulfonyl) amide	41.43	41.24	0.19
n-Dodecanal	22.83	23.08	-0.25
n-Dodecylamine	24.26	24.23	0.03
n-Dodecylmercaptan	25.98	25.91	0.07
N-Dodecylpyridinium bis(trifluoromethanesulfonyl) amide	45.06	44.91	0.15
Neohexane	11.96	11.85	0.11
Neomenthol	18.92	18.87	0.05
Neopentylbenzene	19.74	19.75	-0.01
Neopentylidenebromide	16.19	16.07	0.12
Neral	19.62	19.30	0.32
Nerol	19.65	19.66	-0.01
N-Ethyl-1,2-ethanediamine	10.97	10.89	0.08
N-Ethyl-1-naphthalenamine	23.18	23.01	0.17
N-Ethyl-1-propanamine	11.26	11.36	-0.10
N-Ethyl-2-methylallylamine	13.27	13.10	0.17
N-Ethyl-2-methylaniline	17.89	17.80	0.09
N-Ethyl-2-methylpyridinium bis(trifluoromethylsulfonyl)amide	28.36	28.36	0.00
N-Ethylaniline	16.04	15.89	0.15
N-Ethylbenzaldehydeimine	17.62	17.43	0.19
N-Ethylformamide	7.87	7.75	0.12
N-Ethylmorpholine	13.37	13.20	0.17
N-Ethylmorpholinium formate	16.28	16.52	-0.24
N-Ethyl-N-methylmorpholinium N-acetylalaninate	25.86	25.91	-0.05
N-Ethyl-N-methylmorpholinium N-acetylisoleucinate	31.16	31.40	-0.24
N-Ethyl-N-methylmorpholinium N-acetylleucinate	31.18	31.40	-0.22
N-Ethyl-N-methylmorpholinium N-acetylvalinate	29.34	29.57	-0.23
N-Fenchylaminotriethylsilane	33.19	33.29	-0.10
n-Heptaldehyde	13.83	13.90	-0.07

n-Heptylacetate	17.95	18.06	-0.11
n-Heptylamine	15.06	15.06	0.00
n-Heptylformate	16.26	16.28	-0.02
n-Heptylnitrite	15.72	16.11	-0.39
n-Hexanoic acid	12.55	12.49	0.06
n-Hexylacetate	16.11	16.22	-0.11
n-Hexylamine	13.20	13.22	-0.02
n-Hexylformate	14.42	14.44	-0.02
N-Hexyl-N-methylmorpholinium N-acetylalaninate	33.07	33.25	-0.18
N-Hexyl-N-methylmorpholinium N-acetylleucinate	38.55	38.74	-0.19
N-Hexyl-N-methylmorpholinium N-acetylvalinate	36.57	36.91	-0.34
Nikethamide	20.43	20.34	0.09
N-Isobutyl-3-sulfopropan-1-aminium hydrogen sulfate	24.91	24.86	0.05
N-Isobutylaniline	19.53	19.55	-0.02
N-Isopropylaminotriethylsilane	22.22	22.17	0.05
N-Isopropylaniline	17.60	17.70	-0.10
Nitrobenzene	13.04	13.16	-0.12
Nitrocyclohexane	13.25	13.18	0.07
Nitroethane	6.78	6.79	-0.01
Nitroisobutane	10.44	10.45	-0.01
Nitromethane	4.95	5.08	-0.13
Nitrophenylmethane	14.53	14.69	-0.16
N-Methyl-1,2-ethylenediamine	9.20	9.07	0.13
N-Methyl-2-furanmethanamine	12.49	12.60	-0.11
N-Methyl-2-pyrrolidone	10.69	10.68	0.01
N-Methylalanine ethylester	13.71	13.88	-0.17
N-Methylaniline	14.06	14.07	-0.01
N-Methylbenzaldehydeimine	15.62	15.61	0.01
N-Methylbenzeneethanamine	17.41	17.44	-0.03
N-Methylcyclohexylamine	14.08	14.17	-0.09
N-Methyldiphenylamine	24.33	24.20	0.13
N-Methylformamide	6.01	5.93	0.08
N-Methylformanilide	15.80	16.06	-0.26
N-Methylmorpholine	11.52	11.38	0.14
N-Methyl-m-toluidine	15.98	15.98	0.00
N-Methyl-N-(2,3-dihydroxypropyl)pyrrolidinium bis(trifluoromethanesulfonyl) amide	29.68	29.76	-0.08
N-Methyl-N-phenyl-difluoroacetamide	17.65	17.80	-0.15
N-Methyl-o-toluidine	16.11	15.98	0.13
N-Methylpiperidine	12.59	12.54	0.05
N-Methylpropargylamine	8.70	8.73	-0.03

N-Methylpropionamide	9.68	9.55	0.13
N-Methylpyrrolidine	10.53	10.71	-0.18
N-Nitrosodibutylamine	18.62	18.65	-0.03
N-Nitrosodiethylamine	11.29	11.31	-0.02
N-Nitrosodihexylamine	25.98	26.00	-0.02
N-Nitrosodimethylamine	7.65	7.67	-0.02
N-Nitrosodipentylamine	22.28	22.33	-0.05
N-Nitrosodipropylamine	14.95	14.98	-0.03
N-Nitroso-N-methyl-N-butylamine	13.16	13.16	0.00
N-Nitroso-N-methyl-N-isobutylamine	13.18	13.15	0.03
N-Nitroso-N-methyl-N-isopropylamine	11.29	11.30	-0.01
N-Nitroso-N-methyl-N-propylamine	11.32	11.33	-0.01
N-Nitrosopiperidine	12.38	12.30	0.08
N-Nitrosopyrrolidine	10.54	10.46	0.08
n-Nonanal	17.53	17.57	-0.04
n-Nonylamine	18.74	18.73	0.01
n-Nonylformate	20.16	19.95	0.21
n-Nonylmercaptan	20.47	20.41	0.06
n-Octanoic acid	16.23	16.17	0.06
N-Octyl-2-pyrrolidone	23.47	23.51	-0.04
n-Octylacetate	19.65	19.90	-0.25
n-Octylamine	16.88	16.89	-0.01
n-Octylformate	18.18	18.11	0.07
N-Octyl-N-methylmorpholinium N-acetylalaninate	36.79	36.92	-0.13
N-Octyl-N-methylmorpholinium N-acetylvalinate	40.48	40.58	-0.10
Nonacosane	54.18	54.07	0.11
Nonadecane	35.78	35.72	0.06
Nonadecylbenzene	45.47	45.46	0.01
Nonane	17.39	17.37	0.02
Nonanedinitrile	17.29	17.20	0.09
Nonanedioic acid	18.67	18.63	0.04
Nonanedioyl dichloride	21.70	21.69	0.01
Nonyl acetate	21.54	21.73	-0.19
Nonyl thiocyanate	22.34	22.32	0.02
Nonylbenzene	26.88	27.10	-0.22
Nonylcyclohexane	27.56	27.51	0.05
Nonylcyclopentane	25.72	25.68	0.04
Nonyloxytrimethylsilane	26.98	26.99	-0.01
Nopinene	17.74	17.37	0.37
Norcarane	12.16	11.97	0.19
Nornicotine	17.11	17.47	-0.36
Norpempidine	17.83	17.80	0.03



Novoldiamine	20.43	20.21	0.22
n-Pentyl-2-mercaptan	13.10	13.06	0.04
N-Phenylethanolamine	16.44	16.45	-0.01
N-Phenyl-N-benzylbenzenemethanamine	35.81	35.51	0.30
N-Phenylpiperidine	20.78	20.70	0.08
n-Propyl acetate	10.67	10.72	-0.05
n-Propyl benzoate	18.71	18.62	0.09
n-Propyl iodide	11.44	11.46	-0.02
n-Propyl trifluoacetate	10.98	10.83	0.15
N-Propyl-2-methylpyridinium bis(trifluoromethylsulfonyl)amide	30.24	30.19	0.05
N-Propylaminotriethylsilane	22.24	22.19	0.05
N-Propylaniline	17.89	17.73	0.16
n-Propylbromoacetate	13.70	13.79	-0.09
n-Propylchloroacetate	12.57	12.62	-0.05
n-Propylformate	8.86	8.93	-0.07
n-Propyliodoacetate	15.75	15.82	-0.07
n-Propylmethacrylate	14.22	14.29	-0.07
n-Propylnitrate	9.53	9.37	0.16
N-Propyl-N-methylmorpholinium N-acetylalaninate	27.58	27.75	-0.17
N-Propyl-N-methylmorpholinium N-acetylleucinate	33.25	33.24	0.01
N-Propyl-N-methylmorpholinium N-acetylvalinate	31.32	31.40	-0.08
n-Propylvinylacetate	14.13	14.27	-0.14
N-t-Butylaminotriethylsilane	24.03	24.00	0.03
N-t-Butylbenzylamine	21.11	21.07	0.04
n-Undecanoic acid	21.39	21.67	-0.28
n-Undecylamine	22.42	22.40	0.02
n-Undecylmercaptan	24.14	24.08	0.06
n-Valeraldehyde	10.10	10.23	-0.13
O,O-Dibutyl butylphosphorus thioxide	30.06	30.24	-0.18
O,O-Dibutylthiophosphoric acid	23.21	23.15	0.06
O,O-Diethyl butylphosphorus thioxide	22.91	22.90	0.01
O,O-diethyl ethylthiophosphinate	19.18	19.23	-0.05
O,O-Diethyl propylphosphorus thioxide	20.99	21.06	-0.07
O,O-Diethylthiophosphoric acid	16.04	15.80	0.24
O,O-Diisobutylthiophosphoric acid	23.33	23.11	0.22
O,O-Diisopropylthiophosphoric acid	19.72	19.48	0.24
O,O-Dimethylthiophosphoric acid	12.34	12.11	0.23
O,O-Dipropyl butylphosphorus thioxide	26.53	26.57	-0.04
O,O-Dipropyl propylphosphorus thioxide	24.71	24.73	-0.02
O,O-Dipropylthiophosphoric acid	19.83	19.48	0.35
O,S-Dimethyldithiocarbonate	13.44	13.44	0.00

o-Cresol	13.07	13.12	-0.05
o-Cresylacetate	16.63	16.87	-0.24
Octadecamethyloctasiloxane	63.50	63.76	-0.26
Octadecane	34.16	33.88	0.28
Octadecanoyl chloride	36.14	36.05	0.09
Octadecyl perfluorobutyrate	42.71	42.33	0.38
Octadecylbenzene	43.72	43.62	0.10
Octadecylcyclohexane	44.12	44.03	0.09
Octadecyltrichlorosilane	42.82	42.85	-0.03
Octafluoronaphthalene	17.64	17.31	0.33
Octahydroindolizine	15.40	15.32	0.08
Octamethylcyclotetrasiloxane	29.60	29.57	0.03
Octamethyltrisiloxane	26.73	26.80	-0.07
Octane	15.52	15.53	-0.01
Octanedioic acid	16.74	16.80	-0.06
Octanoic anhydride	30.91	30.92	-0.01
Octanoyl chloride	17.59	17.70	-0.11
Octodrine	16.93	16.85	0.08
Octyl butanoate	23.61	23.57	0.04
Octyl nitrite	18.25	17.95	0.30
Octyl octanoate	31.02	30.91	0.11
Octyl phenyl ether	25.79	25.96	-0.17
Octyl propanoate	21.67	21.73	-0.06
Octyl thiocyanate	20.49	20.49	0.00
Octylbenzene	25.23	25.27	-0.04
Octylcyanide	17.28	17.28	0.00
Octylcyclohexane	25.72	25.68	0.04
Octylcyclopentane	23.89	23.84	0.05
Octyloxytrimethylsilane	25.14	25.15	-0.01
Octylphosphinic dichloride	23.13	23.14	-0.01
o-Cumenol	16.52	16.78	-0.26
O-Ethyl 2-methylpropanoic imino ester	13.93	13.56	0.37
O-Ethyl 4-methylpentanoic imino ester	16.98	17.23	-0.25
O-Ethyl butanoic imino ester	13.66	13.58	0.08
O-Ethyl hexanoic imino ester	17.03	17.25	-0.22
O-Ethyl pentanoic imino ester	15.61	15.41	0.20
O-Ethyl propanoic imino ester	11.83	11.74	0.09
O-Hexyl S-propenylxanthate	26.04	26.26	-0.22
O-Methyl S-propenylxanthate	16.84	17.07	-0.23
Orthoformic acid trimethyl ester	10.05	10.17	-0.12
o-Toluenesulfonyl chloride	18.16	18.07	0.09
o-Toluidine	14.01	14.03	-0.02

o-Tolylamino(diethylamino)borane	25.16	25.10	0.06
Oxacyclohexadecan-2-one	27.88	28.22	-0.34
Oxalylchloride	8.82	8.85	-0.03
Oxepane	11.76	11.68	0.08
Oxetane	6.20	6.18	0.02
Oxirane	4.36	4.34	0.02
Oxiranecarboxaldehyde	6.43	6.39	0.04
Palmitic acid	31.07	30.85	0.22
Paracetamol	16.76	16.70	0.06
Paramethadione	14.91	14.93	-0.02
Parasorbic acid	11.57	11.63	-0.06
Pargyline	20.37	20.48	-0.11
Patchouli alcohol	26.30	26.31	-0.01
p-Cresol	13.03	13.12	-0.09
p-Cymene	17.97	17.98	-0.01
Pelargonic acid	18.06	18.00	0.06
Pelletierine	16.18	16.10	0.08
Pempidine	19.46	19.83	-0.37
Pentachloroethane	14.10	14.18	-0.08
Pentacosane	46.81	46.73	0.08
Pentadecane	28.39	28.38	0.01
Pentadecanedioic acid	29.60	29.65	-0.05
Pentadecylamine	29.78	29.74	0.04
Pentadecylbenzene	38.11	38.11	0.00
Pentadecylcyclohexane	38.60	38.53	0.07
Pentaerythritol tetrakis(2-mercaptoacetate)	39.26	39.64	-0.38
Pentaethylbenzene	28.99	29.22	-0.23
Pentafluoroanisole	12.99	12.90	0.09
Pentafluorobenzene	10.45	10.31	0.14
Pentafluorophenol	10.69	11.02	-0.33
Pentamethylbenzene	19.70	20.05	-0.35
Pentane	10.02	10.02	0.00
Pentanedinitrile	9.88	9.86	0.02
Pentanedioic acid	11.23	11.29	-0.06
Pentanedioyl dichloride	14.19	14.35	-0.16
Pentanenitrile	9.91	9.94	-0.03
Pentanoic acid	10.65	10.66	-0.01
Pentanoic anhydride	20.10	19.91	0.19
Pentasilane	24.10	24.09	0.01
Pentyl 1-naphthaleneacetate	31.11	31.24	-0.13
Pentyl 1-naphthoate	29.58	29.41	0.17
Pentyl 1-naphthylketone	28.85	28.82	0.03

Pentyl 2-naphthaleneacetate	31.22	31.24	-0.02
Pentyl 2-naphthoate	29.81	29.41	0.40
Pentyl 2-thiophenecarboxylate	21.89	21.68	0.21
Pentyl benzoate	22.43	22.29	0.14
Pentyl butyrate	17.93	18.06	-0.13
Pentyl cyclohexyloxy dithiophosphinic acid	30.54	30.52	0.02
Pentyl dichloro phosphorus oxide	17.38	17.26	0.12
Pentyl dichloro phosphorus thioxide	20.47	20.55	-0.08
Pentyl ethoxy dithiophosphinic acid	24.04	24.03	0.01
Pentyl heptanoate	23.61	23.57	0.04
Pentyl hexanoate	21.71	21.73	-0.02
Pentyl hexyloxy dithiophosphinic acid	31.44	31.37	0.07
Pentyl hydroperoxide	11.52	11.51	0.01
Pentyl isopropoxy dithiophosphinic acid	25.94	25.87	0.07
Pentyl methoxy dithiophosphinic acid	22.25	22.18	0.07
Pentyl nitrite	12.34	12.44	-0.10
Pentyl nonanoate	27.59	27.24	0.35
Pentyl octanoate	25.29	25.40	-0.11
Pentyl pentanoate	19.86	19.90	-0.04
Pentyl phenyl sulfide	23.08	23.05	0.03
Pentyl propoxy dithiophosphinic acid	25.99	25.86	0.13
Pentyl salicylate	23.05	22.99	0.06
Pentylcyclohexane	20.20	20.17	0.03
Pentylcyclopentane	18.36	18.34	0.02
Pentyldichloroborane	15.65	15.62	0.03
Pentyloxybenzene	20.47	20.45	0.02
Pentyloxytrimethylsilane	19.63	19.65	-0.02
Pentylphosphinic dichloride	17.76	17.63	0.13
Pentyltrichlorosilane	19.34	18.99	0.35
Peonol	17.99	17.65	0.34
Perchlorocyclopentadiene	20.75	20.64	0.11
Perchlorocyclopentene	24.42	24.45	-0.03
Perfluoro-2-methylpentane	12.51	12.44	0.07
Perfluorobutanoic acid	9.46	9.24	0.22
Perfluorocyclobutene	7.45	7.48	-0.03
Perfluorocyclohexene	11.42	11.46	-0.04
Perfluoroheptane	14.63	14.67	-0.04
Perfluorohexane	12.52	12.68	-0.16
Perfluoromethylcyclohexane	13.85	13.65	0.20
Perfluorotoluene	12.65	12.33	0.32
Perfluoro-trans-decalin	18.49	18.59	-0.10
Perfluorotributylamine	25.67	25.78	-0.11

Perfluorotripropylamine	19.83	19.82	0.01
Perhydrofluorene	22.03	22.10	-0.07
Perhydrophenanthrene	23.80	23.93	-0.13
Perillaldehyde	18.38	18.40	-0.02
Phenanthrene	24.47	24.75	-0.28
Phenethyl alcohol	14.72	14.81	-0.09
Phenethyl propionate	20.20	20.45	-0.25
Pheniramine	30.19	30.18	0.01
Phenol	11.12	11.21	-0.09
Phenoxyacetylene	13.83	14.17	-0.34
Phenoxytriethylsilane	25.56	25.59	-0.03
Phenoxytrimethylsilane	20.28	20.16	0.12
Phenoxytripropylsilane	31.08	31.10	-0.02
Phenyl 2-tolyl propoxyborine	30.57	30.54	0.03
Phenyl chloroacetate	16.70	16.86	-0.16
Phenyl chlorofluorophosphate	15.90	15.97	-0.07
Phenyl di(sec-butoxy)borine	28.32	28.40	-0.08
Phenyl di(sec-octoxy)borine	43.03	43.08	-0.05
Phenyl dibutoxyborine	28.27	28.39	-0.12
Phenyl diethoxyborine	20.96	21.05	-0.09
Phenyl diisobutoxyborine	28.32	28.36	-0.04
Phenyl dimethoxyborine	17.22	17.35	-0.13
Phenyl dipropoxyborine	24.74	24.72	0.02
Phenyl ethoxy 2-(ethoxycarbonyl)propyl phosphorus oxide	29.71	29.66	0.05
Phenyl ethoxy 2-(methoxycarbonyl)ethyl phosphorus oxide	26.06	25.99	0.07
Phenyl ethoxy 2-(methoxycarbonyl)propyl phosphorus oxide	27.96	27.81	0.15
Phenyl ethoxy 2-(propoxycarbonyl)propyl phosphorus oxide	31.45	31.49	-0.04
Phenyl hexoxy 2-(methoxycarbonyl)propyl phosphorus oxide	35.37	35.15	0.22
Phenyl isobutoxy 2-(methoxycarbonyl)propyl phosphorus oxide	31.54	31.47	0.07
Phenyl n-propyl sulfide	19.44	19.38	0.06
Phenyl O-ethyl phosphonic acid	18.48	18.42	0.06
Phenyl O-heptyl phosphonic acid	27.48	27.60	-0.12
Phenyl O-hexyl phosphonic acid	25.52	25.77	-0.25
Phenyl O-isobutyl phosphonic acid	21.94	22.08	-0.14
Phenyl O-isopropyl phosphonic acid	20.03	20.26	-0.23
Phenyl O-methyl phosphonic acid	16.30	16.58	-0.28
Phenyl O-nonyl phosphonic acid	31.24	31.27	-0.03

Phenyl O-octyl phosphonic acid	29.33	29.44	-0.11
Phenyl propanoate	16.72	16.80	-0.08
Phenyl vinyl ether	14.88	14.66	0.22
Phenyl-2-thienylmethanone	21.99	21.66	0.33
Phenylacetaldehyde	14.22	14.46	-0.24
Phenylacetate	14.81	14.96	-0.15
Phenylacetone	16.05	16.20	-0.15
Phenylacetonitrile	13.86	14.17	-0.31
Phenylacetyl chloride	16.27	16.42	-0.15
Phenylamino(diethylamino)borane	23.33	23.19	0.14
Phenylbis(2-methylallyl)phosphine	29.00	29.04	-0.04
Phenylboron dichloride	16.51	16.38	0.13
Phenylchloroacetylene	15.76	15.81	-0.05
Phenylcyclohexane	20.91	20.73	0.18
Phenyldiallylphosphine	25.06	25.31	-0.25
Phenyldibutylcarbinol	27.50	27.64	-0.14
Phenyldichlorofluoromethane	16.37	16.26	0.11
Phenylisocyanate	13.46	13.30	0.16
Phenylphosphine	14.50	14.33	0.17
Phenylphosphorous diaziridide	23.30	23.35	-0.05
Phenylpropylboronic acid	18.39	18.31	0.08
Phenylpropylboronic anhydride	35.79	36.09	-0.30
Phenylpropylether	16.80	16.78	0.02
Phenylsilane	14.84	14.70	0.14
Phenyltri(2-octyloxy)silane	59.39	59.40	-0.01
Phenyltri(cyclohexyloxy)silane	45.86	45.84	0.02
Phenyltrichlorosilane	19.39	19.55	-0.16
Phenyltrifluorosilane	13.12	13.17	-0.05
Phenyltriisopentyloxysilane	42.91	42.82	0.09
Phenyltrimethylsilane	19.77	19.90	-0.13
Phlorol	14.90	14.96	-0.06
Phosphamidon	27.41	27.07	0.34
Phosphoric acid	4.86	5.12	-0.26
Phosphoric acid ethylester	8.97	8.97	0.00
Phthaloyl chloride	18.70	18.65	0.05
Phytol	37.86	38.01	-0.15
Pimelonitrile	13.64	13.53	0.11
Pinacolone	11.91	11.96	-0.05
Piperidine	10.60	10.51	0.09
Piperitenone	18.80	18.39	0.41
Piperitone	18.52	18.38	0.14
p-Isopropenylisopropylbenzene	21.75	21.56	0.19

Pivalaldehyde	9.96	10.22	-0.26
Pivalic acid chloride	11.90	12.18	-0.28
Pivalone	17.29	17.46	-0.17
Pivalonitrile	10.00	9.93	0.07
Pivalophenone	19.93	19.86	0.07
Placidyl	15.06	15.21	-0.15
p-Menthadiene	18.02	18.19	-0.17
p-Menthane	18.36	18.31	0.05
Prehnitene	17.88	18.14	-0.26
Pristane	35.79	35.66	0.13
Propanal	6.43	6.56	-0.13
Propanal oxime	8.06	8.14	-0.08
Propanamide	7.59	7.60	-0.01
Propandioic acid	7.56	7.62	-0.06
Propane	6.29	6.35	-0.06
Propane-1,2-dinitrite	11.33	11.19	0.14
Propane-1,2-dithiol	12.31	12.43	-0.12
Propane-1,3-dithiol	12.48	12.44	0.04
Propanedioyl dichloride	10.62	10.68	-0.06
Propanenitrile	6.25	6.27	-0.02
Propanoic acid	6.90	6.99	-0.09
Propanoic anhydride	12.47	12.57	-0.10
Propanolamine	8.33	8.27	0.06
Propanone	6.46	6.46	0.00
Propanoyl chloride	8.41	8.52	-0.11
Propargyl acetate	9.83	9.91	-0.08
Propargyl aldehyde	5.72	5.75	-0.03
Propargyl propionate	11.65	11.75	-0.10
Propargylamine	7.28	6.91	0.37
Propenal	6.44	6.44	0.00
Propham	20.41	20.32	0.09
Propiolic acid	6.31	6.18	0.13
Propoxyacetylene	9.86	9.93	-0.07
Propoxydichloromethylsulfenyl chloride	17.99	18.02	-0.03
Propyl 1-naphthaleneacetate	27.45	27.57	-0.12
Propyl 1-naphthoate	25.86	25.74	0.12
Propyl 1-naphthylketone	25.10	25.15	-0.05
Propyl 2-hydroxybenzoate	19.65	19.32	0.33
Propyl 2-naphthaleneacetate	27.58	27.57	0.01
Propyl 2-naphthoate	26.11	25.74	0.37
Propyl 2-thiophenecarboxylate	18.21	18.01	0.20
Propyl 3-chloropropanoate	14.44	14.46	-0.02

Propyl 4-toluenesulfonate	21.83	21.87	-0.04
Propyl butyrate	14.33	14.39	-0.06
Propyl chloroformate	10.89	10.87	0.02
Propyl dichloroacetate	14.61	14.55	0.06
Propyl hexanoate	18.19	18.06	0.13
Propyl hydrocinnamate	22.12	22.29	-0.17
Propyl isobutanoate	14.00	14.37	-0.37
Propyl isocyanate	8.95	9.16	-0.21
Propyl isothiocyanate	12.23	12.16	0.07
Propyl isovalerate	16.19	16.21	-0.02
Propyl N,N-diethylamino phosphorusoxy chloride	20.20	20.15	0.05
Propyl N,N-diethylamino phosphorusoxy fluoride	17.79	17.79	0.00
Propyl nitrite	8.81	8.77	0.04
Propyl octanoate	21.54	21.73	-0.19
Propyl phenylacetate	20.30	20.45	-0.15
Propyl phosphorusoxy dichloride	13.64	13.58	0.06
Propyl propanoate	12.49	12.55	-0.06
Propyl propylxanthate	20.89	20.88	0.01
Propyl thiocyanate	11.25	11.31	-0.06
Propyl trichloroacetate	16.56	16.55	0.01
Propyl valerate	16.16	16.22	-0.06
Propyl vinyl ether	10.57	10.42	0.15
Propylallene	11.72	11.84	-0.12
Propylammonium nitrate	11.41	11.39	0.02
Propylbenzenesulfonate	19.90	19.96	-0.06
Propylbutoxyphosphinic chloride	17.87	17.87	0.00
Propylcyclohexane	16.52	16.50	0.02
Propylcyclohexylketone	18.57	18.44	0.13
Propylcyclopentane	14.70	14.67	0.03
Propylene	6.26	6.23	0.03
Propylenecarbonate	8.48	8.62	-0.14
Propylenediamine	8.92	9.05	-0.13
Propyleneglycol dinitrate	12.28	12.40	-0.12
Propylhexedrine	19.83	19.66	0.17
Propyliodoacetylene	14.18	14.27	-0.09
Propylisobutoxyphosphinic chloride	17.73	17.85	-0.12
Propylisopropoxyphosphinic chloride	16.09	16.04	0.05
Propylphosphonyl difluoride	9.36	9.39	-0.03
Propylpropoxyphosphinic chloride	15.98	16.03	-0.05
Propylsulfinyl chloride	12.11	12.04	0.07
Propylsulfonyl fluoride	9.80	10.17	-0.37
Propyltrichlorosilane	15.25	15.32	-0.07



Propyltriisothiocyanatosilane	27.23	27.39	-0.16
Pseudopelletierine	17.11	17.25	-0.14
p-Toluidine	14.14	14.03	0.11
Pulegone	18.57	18.42	0.15
p-Xylyldiallylphosphine	28.93	29.13	-0.20
Pyrazine	8.98	8.69	0.29
Pyrene	28.77	28.37	0.40
Pyridazine	8.77	8.78	-0.01
Pyridine	9.54	9.60	-0.06
Pyrimidine	8.53	8.44	0.09
Pyrrole	8.18	8.40	-0.22
Pyrrolidine	8.71	8.68	0.03
Pyrvaldehyde	6.63	6.67	-0.04
Pyruvic acid	7.32	7.10	0.22
Quinoline	16.53	16.57	-0.04
R-11	22.57	22.83	-0.26
Refrigerant 115	6.58	6.60	-0.02
Refrigerant 216	10.51	10.45	0.06
Rhodinol	19.68	19.65	0.03
Ricinelaidic acid	35.03	35.00	0.03
Safranal	18.84	18.45	0.39
Safrole	18.29	18.39	-0.10
s-Butyl ethyl ether	12.51	12.53	-0.02
s-Butyl pentanoate	17.95	18.06	-0.11
s-Butyl propionate	14.30	14.39	-0.09
s-Butylacetate	12.44	12.56	-0.12
s-Butylbenzene	17.85	17.91	-0.06
S-Butyl-dimethylthioformamidium bis(trifluoromethylsulfonyl) amide	31.42	31.32	0.10
S-Butyl-dimethylthioformamidium difluorooxalylborate	25.14	25.01	0.13
s-Butylethylamine	13.27	13.17	0.10
s-Butylformate	10.76	10.77	-0.01
s-Butylmethylether	10.61	10.69	-0.08
s-Butylnitrate	11.19	11.21	-0.02
s-Butylnitrite	10.62	10.61	0.01
s-Butyl-t-butylether	15.99	16.19	-0.20
Sebaconitrile	19.07	19.04	0.03
sec-Amyl acetate	14.25	14.39	-0.14
sec-Butyl hydroperoxide	9.63	9.68	-0.05
S-Ethyl thioacetate	11.51	11.46	0.05

S-Ethyl-dimethylthioformamidium bis(trifluoromethylsulfonyl) amide	27.68	27.65	0.03
S-Ethyl-dimethylthioformamidium difluorooxalylborate	21.35	21.34	0.01
S-Ethyl-dimethylthioformamidium trifluoromethylsulfonate	21.25	20.99	0.26
S-Methyl-dimethylthioformamidium bis(trifluoromethylsulfonyl) amide	25.75	25.73	0.02
S-Methyl-dimethylthioformamidium trifluoromethylsulfonate	19.15	19.07	0.08
Solanone	24.95	24.61	0.34
Sorbic alcohol	12.72	12.26	0.46
Sparteine	28.20	27.93	0.27
s-Phenethyl alcohol	14.69	14.82	-0.13
Spiro[5.5]undecane	19.28	19.33	-0.05
S-Propylthioacetate	13.27	13.30	-0.03
Squalene	55.69	55.60	0.09
S-sec-Butyl thioacetate	15.18	15.13	0.05
S-t-Butyl thiolacetate	15.15	15.28	-0.13
Stearic acid	34.47	34.52	-0.05
Stearyl mercaptan	37.02	36.92	0.10
Styrene	14.46	14.13	0.33
Styrene oxide	14.12	14.08	0.04
Suberone	12.83	12.95	-0.12
Suberonitrile	15.28	15.36	-0.08
Succinonitrile	8.10	8.02	0.08
Succinyl chloride	12.43	12.52	-0.09
Sucrose octaacetate	58.21	57.96	0.25
Sulcatol	16.00	16.04	-0.04
Sulcatone	15.56	15.59	-0.03
Sulfolane	10.70	10.81	-0.11
Sulfotep	30.09	30.39	-0.30
t-Amyl mercaptan	13.37	13.21	0.16
t-Amyl t-butyl disulfide	23.91	24.05	-0.14
t-Amylhydroperoxide	11.48	11.49	-0.01
t-Butoxytriethylsilane	23.21	23.23	-0.02
t-Butoxytrimethylsilane	17.83	17.79	0.04
t-Butoxytripropylsilane	28.81	28.73	0.08
t-Butyl acrylate	14.35	14.25	0.10
t-Butyl isocyanate	11.13	10.97	0.16
t-Butyl vinyl ether	12.30	12.23	0.07
t-Butylacetate	12.47	12.53	-0.06
t-Butylacetylene	11.22	11.04	0.18

t-Butylamine	9.62	9.52	0.10
t-Butylbenzene	17.83	17.92	-0.09
t-Butylcyclohexane	18.28	18.33	-0.05
t-Butylformamide	11.54	11.40	0.14
t-Butylformate	10.73	10.75	-0.02
t-Butylhydroperoxide	9.70	9.65	0.05
t-Butylmercaptan	11.46	11.38	0.08
t-Butylnitrite	10.61	10.59	0.02
t-Butyl-t-amylperoxide	18.99	18.96	0.03
TEPP	24.47	24.42	0.05
Terpinen-4-ol	18.71	18.83	-0.12
Terpinolene	18.04	18.28	-0.24
tert-Butyl 3-oxobutanoate	16.20	16.31	-0.11
Tetra(1H,1H,3H-perfluoropropyl)silicate	28.62	28.58	0.04
Tetra(1H,1H,5H-perfluoropentyl)silicate	44.38	44.47	-0.09
Tetra(2-ethylbutyl) silicate	49.76	50.11	-0.35
Tetra(diethylamino)silane	38.58	38.74	-0.16
Tetra(dimethylamino)silane	24.30	24.18	0.12
Tetra-2-butoxysilane	35.87	35.51	0.36
Tetra-2-methyl-1-propoxysilane	35.23	35.43	-0.20
Tetra-2-pentoxysilane	43.20	42.85	0.35
Tetra-3-methyl-1-butoxysilane	42.51	42.77	-0.26
Tetrabutoxysilane	35.23	35.49	-0.26
Tetrabutylphosphonium acetate	38.54	38.58	-0.04
Tetrabutylphosphonium formate	37.09	36.88	0.21
Tetrabutylphosphonium propanoate	40.50	40.42	0.08
Tetracene	32.27	31.87	0.40
Tetrachloroethylene	12.03	12.13	-0.10
Tetrachlorothiophene	17.46	17.47	-0.01
Tetracosamethylhendecasiloxane	86.12	85.94	0.18
Tetracosane	44.83	44.90	-0.07
Tetracosanoic acid	45.88	45.53	0.35
Tetradecamethylcycloheptasiloxane	51.86	51.75	0.11
Tetradecamethylhexasiloxane	48.94	48.98	-0.04
Tetradecane	26.69	26.54	0.15
Tetradecanoic acid	27.13	27.18	-0.05
Tetradecanoic anhydride	53.22	52.95	0.27
Tetradecyl trihexylphosphonium bis(trifluoromethylsulfonyl)amide	76.33	76.33	0.00
Tetradecyl trihexylphosphonium chloride	65.93	66.10	-0.17
Tetradecylbenzene	36.27	36.28	-0.01
Tetradecylcyclohexane	36.75	36.69	0.06

Tetraethoxymethane	19.69	19.76	-0.07
Tetraethoxysilane	21.14	20.81	0.33
Tetraethylmethane	17.09	17.36	-0.27
Tetraethylsilane	19.17	19.27	-0.10
Tetraethylurea	19.87	19.99	-0.12
Tetraglycol	18.61	18.66	-0.05
Tetrahexoxysilane	50.54	50.18	0.36
Tetrahydro-2,5-dimethoxyfuran	12.94	12.87	0.07
Tetrahydro-2H-pyran-2-methanol	12.23	12.24	-0.01
Tetrahydro-2H-pyran-2-one	9.63	9.87	-0.24
Tetrahydro-3-furanol	8.61	8.57	0.04
Tetrahydro-3-methyl-2H-thiopyran	14.12	14.14	-0.02
Tetrahydro-4H-pyran-4-one	9.88	9.95	-0.07
Tetrahydrodicyclopentadiene	16.62	16.59	0.03
Tetrahydrofuran	7.88	8.01	-0.13
Tetrahydrofurfuryl acetate	14.04	14.21	-0.17
Tetrahydrofurfuryl alcohol	10.38	10.41	-0.03
Tetrahydrofurfuryl methacrylate	17.62	17.79	-0.17
Tetrahydrofurfurylamine	11.16	11.21	-0.05
Tetrahydromyrcenol	19.88	19.72	0.16
Tetrahydropyran	9.80	9.85	-0.05
Tetraisobutylsilane	34.09	33.89	0.20
Tetraisopropoxysilane	28.07	28.17	-0.10
Tetraisopropylsilane	26.53	26.69	-0.16
Tetramethyl orthocarbonate	12.35	12.37	-0.02
Tetramethylene glycol	9.37	9.31	0.06
Tetramethylethene	11.73	11.84	-0.11
Tetramethyloxirane	11.76	11.64	0.12
Tetramethylsilane	11.87	12.02	-0.15
Tetramethyltetraphenylcyclotetrasiloxane	61.17	61.09	0.08
Tetramethylurea	12.76	12.71	0.05
Tetramethoxysilane	13.28	13.42	-0.14
Tetraoctoxysilane	64.97	64.86	0.11
Tetrapentoxysilane	42.57	42.83	-0.26
Tetrapropoxymethane	27.19	27.10	0.09
Tetrapropoxysilane	28.01	28.15	-0.14
Tetrasilane	19.38	19.31	0.07
Tetravinylsilane	18.58	18.67	-0.09
Thiamorpholine	11.77	11.82	-0.05
Thianaphthene	16.64	16.34	0.30
Thiane	12.22	12.32	-0.10
Thiepane	13.77	14.15	-0.38

Thietane	8.62	8.65	-0.03
Thiirane	6.84	6.81	0.03
Thioacetic acid	7.84	7.60	0.24
Thioanisole	15.64	15.63	0.01
Thioglycerol	10.58	10.52	0.06
Thiolactic acid	10.03	10.02	0.01
Thiolane	10.37	10.48	-0.11
Thiolane 1-oxide	10.77	10.83	-0.06
Thiophene	9.66	9.83	-0.17
Thiophos	28.43	28.21	0.22
Thujone	17.77	17.56	0.21
Tiglic acid	10.70	10.61	0.09
Tiglic aldehyde	10.24	10.18	0.06
t-Nonylmercaptan	20.32	20.55	-0.23
t-Pentylbenzene	19.62	19.75	-0.13
trans-(1-Methyl-1-propenyl)benzene	18.06	17.87	0.19
trans,trans-2,4-Hexadiene	12.06	11.70	0.36
trans-1,2-Bis(trimethylsilyl)-3,3-dichlorocyclopropane	28.15	27.99	0.16
trans-1,2-Dibromocyclohexane	17.06	17.19	-0.13
trans-1,2-Dibromoethene	10.53	10.42	0.11
trans-1,2-Dichloroethylene	8.15	8.16	-0.01
trans-1,2-Dichloropropene	9.95	10.08	-0.13
trans-1,2-Dimethylcyclohexane	14.72	14.65	0.07
trans-1,2-Dimethylcyclopentane	12.97	12.82	0.15
trans-1,2-Dimethylcyclopropane	9.49	9.14	0.35
trans-1,2-Divinylcyclobutane	14.60	14.41	0.19
trans-1,3,5-Trimethylcyclohexane	16.61	16.47	0.14
trans-1,3-Dichloropropene	10.14	10.04	0.10
trans-1,3-Dimethylcyclohexane	14.50	14.65	-0.15
trans-1,3-Dimethylcyclopentane	12.97	12.82	0.15
trans-1,4-Dichloro-2-butene	12.05	11.92	0.13
trans-1,4-Dimethylcyclohexane	14.57	14.65	-0.08
trans-1,4-Hexadiene	11.62	11.66	-0.04
trans-1-Bromo-1-butene	10.94	11.10	-0.16
trans-1-Chloro-1-butene	10.08	9.97	0.11
trans-1-Chloropropene	7.96	8.13	-0.17
trans-1-Ethyl-2-methylcyclopentane	14.77	14.65	0.12
trans-1-Ethyl-3-methylcyclopentane	14.73	14.65	0.08
trans-1-Ethyl-4-methylcyclohexane	16.59	16.49	0.10
trans-1-Methyl-2-propylcyclopentane	16.63	16.49	0.14
trans-2,2-Dimethyl-3-hexene	15.63	15.44	0.19

trans-2,3-Epoxybutane	8.14	8.02	0.12
trans-2-Bromo-2-butene	11.01	11.05	-0.04
trans-2-Butene	8.49	8.11	0.38
trans-2-Butene-1,4-diol	9.20	9.23	-0.03
trans-2-Chloro-2-butene	9.92	10.06	-0.14
trans-2-Hepten-1-ol	14.18	14.18	0.00
trans-2-Heptene	13.59	13.62	-0.03
trans-2-Heptenoic acid	14.29	14.25	0.04
trans-2-Hexen-1-ol	12.18	12.34	-0.16
trans-2-Hexen-1-ol, acetate	16.12	16.15	-0.03
trans-2-Hexenal	12.26	11.99	0.27
trans-2-Hexene	11.84	11.78	0.06
trans-2-Methyl-1,3-pentadiene	12.08	11.69	0.39
trans-2-Methyl-2-pentenoic acid	12.50	12.44	0.06
trans-2-Methyl-3-hexene	13.77	13.60	0.17
trans-2-Methylcyclohexanol	13.45	13.39	0.06
trans-2-Nonenoic acid	17.98	17.92	0.06
trans-2-Octenal	15.89	15.66	0.23
trans-2-Octene	15.42	15.45	-0.03
trans-2-Octenoic acid	16.15	16.09	0.06
trans-2-Penten-1-ol	10.50	10.50	0.00
trans-2-Pentene	10.00	9.95	0.05
trans-2-Pentenoic acid	10.64	10.58	0.06
trans-2-Undecene	20.95	20.96	-0.01
trans-3,4-Dimethyl-2-pentene	13.62	13.63	-0.01
trans-3,7-Dimethyl-2,6-octadien-1-ol formate	22.02	21.68	0.34
trans-3-heptene	13.64	13.62	0.02
trans-3-Heptenoic acid	14.29	14.25	0.04
trans-3-Hexene	11.79	11.78	0.01
trans-3-Hexenoic acid	12.45	12.42	0.03
trans-3-Methyl-3-hexene	13.70	13.64	0.06
trans-3-Methylcyclohexanol	13.42	13.39	0.03
trans-3-Octene	15.50	15.45	0.05
trans-3-Penten-1-yne	9.44	9.14	0.30
trans-3-Pentenitrile	9.76	9.86	-0.10
trans-3-Phenyl-2-propen-1-ol	17.00	16.57	0.43
trans-4,4-Dimethyl-2-pentene	13.64	13.61	0.03
trans-4-Hexen-1-ol	12.30	12.34	-0.04
trans-4-Methyl-2-hexene	13.70	13.60	0.10
trans-4-Methylcyclohexanol	13.41	13.39	0.02
trans-4-Octene	15.48	15.45	0.03
trans-4-Undecene	20.98	20.96	0.02

trans-5-Decene	19.18	19.12	0.06
trans-5-Methyl-2-(1-methylvinyl)cyclohexanone	18.22	18.33	-0.11
trans-5-Methyl-2-hexene	13.73	13.60	0.13
trans-5-Octenoic acid	16.01	16.09	-0.08
trans-5-Undecene	21.01	20.96	0.05
trans-Chlorobromoethylene	9.28	9.29	-0.01
trans-Cinnamyl acetate	20.82	20.37	0.45
trans-Citral	19.57	19.30	0.27
trans-Crotonitrile	8.21	8.03	0.18
trans-Cyclohexane-1,2-dinitrite	15.51	15.86	-0.35
trans-Cyclooctene	14.48	14.60	-0.12
trans-Decalin	17.64	17.47	0.17
trans-Geraniol	19.41	19.66	-0.25
trans-Hydrindan	15.69	15.64	0.05
trans-Octahydro-1(2H)-naphthalenone	17.54	17.58	-0.04
Tri(1,2,2-trimethylpropoxy)borine	37.11	37.37	-0.26
Tri(1,3-dichloro-2-propoxy)borine	32.16	32.29	-0.13
Tri(1-chloroethoxy)borine	21.01	21.21	-0.20
Tri(1-ethoxycarbonylethoxy)borine	34.06	33.97	0.09
Tri(1-methoxyethoxy)borine	22.76	22.65	0.11
Tri(2-ethoxycarbonylethoxy)borine	33.68	33.96	-0.28
Tri(2-pentoxy)borine	31.76	31.89	-0.13
Tri(butylthio)borane	34.67	34.63	0.04
Tri(ethoxycarbonylmethoxy)borine	28.20	28.45	-0.25
Tri(ethoxyethyl) phosphate	29.71	29.69	0.02
Tri(methoxyethyl) phosphate	24.17	24.15	0.02
Tri(propylthio)borane	29.12	29.12	0.00
Tri(t-butoxy)borine	26.47	26.31	0.16
Triallylamine	18.08	18.51	-0.43
Tribromoethylene	13.34	13.44	-0.10
Tributoxymethane	26.76	26.72	0.04
Tributyl borate	26.42	26.37	0.05
Tributyl citrate	36.53	36.50	0.03
Tributyl phosphate	27.60	27.68	-0.08
Tributyl phosphite	27.80	28.11	-0.31
Tributylamine	24.42	24.39	0.03
Tributylisothiocyanatosilane	32.52	32.35	0.17
Tributylmethylammonium bis(trifluoromethylsulfonyl)amide	38.68	38.66	0.02
Tributylphosphine	27.15	27.05	0.10
Tributylsilane	26.76	26.62	0.14
Tributylsilanol	26.87	26.94	-0.07

Tributylsilylamine	27.59	27.66	-0.07
Tricaprilin	52.38	52.49	-0.11
Trichloro-2-phenoxyethylsilane	23.96	23.91	0.05
Trichloroacetaldehyde diethylacetal	18.95	18.97	-0.02
Trichloroacetic acid	11.01	10.99	0.02
Trichloroacetic anhydride	20.72	20.57	0.15
Trichloroacetonitrile	10.49	10.27	0.22
Trichloroacetylchloride	12.40	12.52	-0.12
Trichloroethylene	10.06	10.14	-0.08
Trichloromethoxybenzene	18.69	18.86	-0.17
Trichloromethylchloroformate	12.91	12.95	-0.04
Trichlorotoluene	18.20	18.25	-0.05
Trichlorovinylsilane	13.30	13.33	-0.03
Tricosane	43.13	43.06	0.07
Tridecanal	24.72	24.91	-0.19
Tridecane	24.74	24.71	0.03
Tridecanonitrile	24.61	24.62	-0.01
Tridecyl borate	59.23	59.41	-0.18
Tridecyl methacrylate	32.33	32.65	-0.32
Tridecyl thiocyanate	29.67	29.66	0.01
Tridecylamine	26.10	26.07	0.03
Tridecylbenzene	34.43	34.44	-0.01
Tridecylcyclohexane	34.92	34.86	0.06
Tridecylmercaptan	27.70	27.75	-0.05
Tridodecylamine	68.57	68.43	0.14
Triethanolamine	15.08	15.05	0.03
Triethoxymethylsilane	18.43	18.47	-0.04
Triethoxypentylsilane	25.75	25.79	-0.04
Triethoxyphenylsilane	26.22	26.35	-0.13
Triethyl 1-propoxyethoxysilane	25.83	25.69	0.14
Triethyl 2,2-diethylhydrazinosilane	25.57	25.61	-0.04
Triethyl 2,2-dimethylhydrazinosilane	21.99	21.97	0.02
Triethyl acetylcitrate	29.18	29.30	-0.12
Triethyl aconitate	25.14	24.90	0.24
Triethyl borate	15.34	15.36	-0.02
Triethyl citrate	25.66	25.49	0.17
Triethyl phosphate	16.56	16.67	-0.11
Triethyl phosphite	17.05	17.10	-0.05
Triethylamine	13.39	13.37	0.02
Triethylammonium acetate	18.54	18.40	0.14
Triethylborane	13.37	13.68	-0.31



Triethyldecylammonium bis(trifluoromethylsulfonyl) amide	44.15	44.04	0.11
Triethyldodecylammonium bis(trifluoromethylsulfonyl) amide	47.85	47.71	0.14
Triethyleneglycol	14.27	14.32	-0.05
Triethylheptylammonium bis(trifluoromethylsulfonyl) amide	38.47	38.54	-0.07
Triethylhexylammonium bis(trifluoromethylsulfonyl) amide	36.75	36.70	0.05
Triethylisothiocyanatosilane	21.35	21.33	0.02
Triethylmethanol	14.14	14.23	-0.09
Triethyloctylammonium bis(trifluoromethylsulfonyl) amide	40.42	40.37	0.05
Triethylphosphine	15.96	16.03	-0.07
Triethylsilane	15.70	15.61	0.09
Triethylsilanol	16.09	15.93	0.16
Triethylsilylamine	16.68	16.65	0.03
Triethylsilyloxytripropylsilane	35.75	35.78	-0.03
Triethylsulfonium bis(trifluoromethylsulfonyl) amide	27.76	27.80	-0.04
Triethyltetradecylammonium bis(trifluoromethylsulfonyl) amide	51.47	51.39	0.08
Triethyltriphenylcyclotrisiloxane	51.20	51.25	-0.05
Trifluoroacetic acid	5.41	5.26	0.15
Trifluoroacetic anhydride	9.45	9.12	0.33
Trifluoroacetoacetic acid ethylester	13.38	13.09	0.29
Trifluoroacetophenone	14.73	14.47	0.26
Trifluoromethoxybenzene	12.84	12.93	-0.09
Triheptyl borate	43.28	42.89	0.39
Triheptyl phosphate	44.21	44.20	0.01
Triheptyl phosphite	44.67	44.63	0.04
Trihexoxymethane	37.93	37.73	0.20
Trihexyl phosphate	38.68	38.69	-0.01
Trihexyl phosphite	39.15	39.12	0.03
Trihexyl tetradecyl phosphonium dicyanamide	69.31	69.41	-0.10
Trihexyl tetradecyl phosphonium trifluoromethylsulfonate	69.64	69.66	-0.02
Trihexylamine	35.43	35.40	0.03
Triisoamylamine	29.86	29.84	0.02
Triisobutoxymethane	26.71	26.67	0.04
Triisobutylamine	24.46	24.34	0.12
Triisobutylborane	24.70	24.64	0.06
Triisooctylamine	46.20	46.36	-0.16
Triisopentoxyborine	31.77	31.83	-0.06

Tri-isopentoxymethane	32.23	32.24	-0.01
Triisopentylborane	30.34	30.15	0.19
Triisopropoxymethane	21.21	21.23	-0.02
Triisopropoxyvinylsilane	25.78	25.65	0.13
Triisopropyl borate	20.82	20.88	-0.06
Triisopropyl phosphate	22.12	22.19	-0.07
Triisopropylethoxysilane	25.20	25.14	0.06
Triisopropylphenylsilane	30.72	30.90	-0.18
Triisopropylphosphite	22.49	22.62	-0.13
Triisopropylsilane	21.24	21.18	0.06
Triisopropylsilyl chloride	22.88	22.82	0.06
Trilaurin	74.35	74.51	-0.16
Trimethoxyborine	9.85	9.82	0.03
Trimethoxymethylsilane	12.78	12.93	-0.15
Trimethoxyphenylsilane	20.74	20.81	-0.07
Trimethoxysilylamine	12.27	12.22	0.05
Trimethyl 1-ethoxyethoxysilane	18.44	18.42	0.02
Trimethyl 1-isopropoxyethoxysilane	20.28	20.26	0.02
Trimethyl 2,2-diethylhydrazinosilane	20.21	20.17	0.04
Trimethyl 2,2-dimethylhydrazinosilane	16.56	16.53	0.03
Trimethyl butylammonium bis(trifluoromethylsulfonyl)amide	27.86	27.89	-0.03
Trimethyl hexylammonium bis(trifluoromethylsulfonyl)amide	31.57	31.57	0.00
Trimethyl octylammonium bis(trifluoromethylsulfonyl)amide	35.27	35.24	0.03
Trimethyl pentylammonium bis(trifluoromethylsulfonyl)amide	29.73	29.73	0.00
Trimethyl phosphate	11.00	11.13	-0.13
Trimethyl propylammonium bis(trifluoromethylsulfonyl)amide	26.02	26.06	-0.04
Trimethyl trimellitate	24.22	23.78	0.44
Trimethylacetic acid	10.68	10.65	0.03
Trimethylamine	8.31	7.92	0.39
Trimethyleneglycol dinitrate	12.32	12.40	-0.08
Trimethylethylene	9.89	9.97	-0.08
Trimethylethylenediamine	13.01	12.92	0.09
Trimethylisothiocyanatosilane	15.91	15.90	0.01
Trimethylphosphite	11.57	11.56	0.01
Trimethylsilanol	10.39	10.49	-0.10
Trimethylsilylaminodimethylphenylsilane	28.18	28.22	-0.04
Trimethylsilylaminodiphenylmethylsilane	36.09	36.10	-0.01
Trimethylsilylaminotriethylsilane	25.77	25.77	0.00

Trimethylsilylaminotrimethoxysilane	21.29	21.34	-0.05
Trimethylsilylaminotriphenylsilane	44.27	43.98	0.29
Trimethylsilyloxytriethylsilane	24.76	24.84	-0.08
Trimethylsilyloxytripropylsilane	30.34	30.34	0.00
Trimethylvinylsilane	13.70	13.68	0.02
Trimyristin	85.86	85.52	0.34
tri-n-Amylphosphate	33.15	33.19	-0.04
Tri-n-octylamine	46.70	46.41	0.29
Tri-n-pentylamine	29.85	29.89	-0.04
Trioctyl borate	48.48	48.40	0.08
Trioctyl phosphite	50.19	50.14	0.05
Tripentoxyborine	31.88	31.88	0.00
Tripentoxymethane	32.18	32.23	-0.05
Tripentyl phosphite	33.77	33.62	0.15
Tripentylsilane	32.32	32.13	0.19
Triphenylphosphite	35.05	34.84	0.21
Tripropionine	24.91	24.96	-0.05
Tripropoxymethane	21.06	21.22	-0.16
Tripropyl borate	20.83	20.87	-0.04
Tripropyl phosphate	22.06	22.17	-0.11
Tripropyl phosphite	22.56	22.61	-0.05
Tripropylamine	18.94	18.88	0.06
Tripropylborane	19.24	19.19	0.05
Tripropylene glycol	21.29	21.68	-0.39
Tripropylsilane	20.91	21.12	-0.21
Triptane	13.53	13.67	-0.14
Tri-p-tolylamine	37.49	37.65	-0.16
Tris(2,4-dimethylphenyl) phosphate	45.73	45.85	-0.12
Tris(2-butoxyethyl) phosphite	41.31	41.13	0.18
Tris(2-chloroethyl) phosphate	22.80	22.38	0.42
Tris(2-chloroethyl) phosphite	22.85	22.81	0.04
Tris(2-ethoxyethyl) phosphite	30.27	30.12	0.15
Tris(2-ethylhexyl) aconitate	58.04	57.89	0.15
Tris(2-hexoxyethyl) phosphite	52.32	52.15	0.17
Tris(2-hydroxyethyl)phosphine	17.71	17.71	0.00
Tris(2-methoxyethyl) phosphite	24.72	24.58	0.14
Tris(2-pentoxyethyl) phosphite	46.83	46.64	0.19
Tris(2-propoxyethyl) phosphite	35.79	35.63	0.16
Tris(4-bromophenyl)amine	40.89	40.95	-0.06
Tris(amylothio)phosphite	42.57	42.50	0.07
Tris(butylothio)phosphite	37.00	37.00	0.00
Tris(dimethylamino)dibutylaminosilane	35.11	35.16	-0.05

Tris(ethylthio)borane	23.55	23.62	-0.07
Tris(ethylthio)phosphite	25.88	25.98	-0.10
Tris(o-tolyl) phosphite	40.35	40.56	-0.21
Tris(propylthio)phosphite	31.47	31.49	-0.02
Tris(p-tolyl) phosphite	40.65	40.56	0.09
Trisilane	14.51	14.54	-0.03
Tritane	31.96	31.87	0.09
Tropacocaine	27.80	27.58	0.22
Tropine	15.68	15.87	-0.19
Undecane	21.03	21.04	-0.01
Undecanedioic acid	22.25	22.31	-0.06
Undecanonitrile	20.72	20.95	-0.23
Undecyl thiocyanate	25.98	25.99	-0.01
Undecylbenzene	30.75	30.77	-0.02
Uracil	10.09	9.70	0.39
Urea	5.15	4.82	0.33
Valeramide	11.57	11.27	0.30
Valerophenone	19.69	19.87	-0.18
Valeryl chloride	11.91	12.19	-0.28
Veratrole	15.68	15.68	0.00
Vinyl acetate	8.79	8.60	0.19
Vinyl tris(2-chloropropoxy)silane	31.44	31.30	0.14
Vinylacetylene	7.31	7.26	0.05
Vinylcyclohexane	14.51	14.54	-0.03
Vinylcyclopentane	12.72	12.71	0.01
Vinyldiethoxymethylsilane	17.87	17.93	-0.06
Vinylformate	6.93	6.81	0.12
Vinylidenechloride	8.10	8.24	-0.14
Vinylidoacetylene	12.60	12.31	0.29
Vinyloxirane	7.75	7.89	-0.14
Vinyltriacetoxysilane	20.04	20.00	0.04
Vinyltriethoxysilane	20.12	20.13	-0.01
Vinyltrimethoxysilane	14.43	14.59	-0.16
Vitamin E	53.40	53.56	-0.16
Vitamin E acetate	57.53	57.30	0.23
Widdrene	25.70	25.74	-0.04
Xibornol	31.30	31.71	-0.41
Ylangene	26.01	25.69	0.32
Z,E-Nepetalactone	17.74	17.94	-0.20