

Name	Refractivity exp.	Refractivity calc	Difference
Tetraisothiocyanatosilane	49.55	69.83	-20.28
1-Butyltetrahydrothiophenium bis(trifluoromethylsulfonyl)amide	59.14	77.28	-18.14
Phthalide	72.84	55.04	17.80
Tributylsilyl bromide	87.75	74.35	13.40
PEG-5 cocomonium methylsulfate	97.54	84.61	12.93
N-Nitroso-N-methylaniline	40.03	28.52	11.51
Dihexylphenylcarbinol	99.72	88.24	11.48
Omethoate	47.40	58.40	-11.00
Amiton	71.39	81.98	-10.59
Demeton-S-methyl	57.04	67.50	-10.46
1-(2-Cyanoethyl)-3-octylimidazolium trifluoromethanesulfonate	95.85	85.71	10.14
Methylhydrazine	13.69	4.29	9.40
3-(2-Cyanoethyl)-1-hexylimidazolium 1,1,1-trifluoromethanesulfonate	85.35	76.45	8.90
2-Phenoxyvinyl bis(dimethylamino) phosphorus oxide	62.86	71.65	-8.79
Bis(perfluorobutyl) 3-methylglutarate	82.57	74.39	8.18
4-Ethoxyazobenzene	78.57	70.47	8.10
Bis(butylthio) 2-phenylethyl borane	102.02	94.23	7.79
Trimethylammonium hydrogen sulfate	26.69	34.30	-7.61
1,2,3,4-Tetrachlorobenzene	38.67	45.80	-7.13
Dimethyldi-2-dodecoxysilane	126.53	133.63	-7.10
2-Ethoxyvinyl bis(diethylamino) phosphorus oxide	67.51	74.52	-7.01
Tetra(1H,1H-perfluoropropyl)silicate	66.78	73.62	-6.84
Dipropylphosphine	46.78	40.09	6.69
1-(2-Cyanoethyl)-3-octylimidazolium benzenesulfonate	99.04	105.62	-6.58
Trimethylammonium acetate	26.93	33.20	-6.27
Di-n-butylsulfoxide	54.12	47.98	6.14
1-(2-Cyanoethyl)-3-octylimidazolium dodecylsulfate	131.08	137.11	-6.03
Hexyl ethoxy S-ethyl dithiophosphinate	68.06	74.08	-6.02
Truxene	114.91	109.41	5.50
trans-Stilbene	65.77	60.38	5.39
2-Phenoxyvinyl bis(1-piperidyl) phosphorus oxide	89.67	94.99	-5.32
L-Glutamic acid 1,5-bis(1-methylethyl) ester dodecyl sulfate	133.53	128.21	5.32
1,6-Bis(7-H-perfluoroheptoxy)hexane	108.93	103.68	5.25
2,5-Diphenyloxazole	70.72	65.53	5.19
2-Iodopentane	43.66	38.49	5.17
1-Ethyltetrahydrothiophenium nitrate	38.21	43.34	-5.13
2-Dimethylaminoethyl dimethylammonium acetate	45.69	50.80	-5.11
Phenazone	57.44	62.54	-5.10
1,1,5,5-Tetra(ethylthio)-pent-2-yne	97.39	92.29	5.10
Triethylammonium hydrogen sulfate	52.66	47.56	5.10
2-Ethyl-3-(2-furyl)acrolein	47.88	42.84	5.04
Hexafluoro-1,3-butadiene	24.06	19.06	5.00
1-Ethoxy-1,3,5-hexatriene	44.83	39.86	4.97
3-(2-Cyanoethyl)-1-hexylimidazolium benzenesulfonate	91.39	96.36	-4.97
Triphenoxisothiocyanatosilane	97.36	102.29	-4.93
N-Ethylpyridinium trifluoroacetate	51.01	46.09	4.92
Dibenzo[b,e]pyridine	64.30	59.40	4.90
3-(2-Cyanoethyl)-1-hexylimidazolium dodecyl sulfate	122.95	127.85	-4.90
Ethyl-bis(butylthio)-thiophosphinate	78.58	83.45	-4.87
3-Bromo-3-chloropentane	33.53	38.31	-4.78
2-Methyl-3-(2-furyl)acrolein	42.93	38.21	4.72
9,10-Anthraquinone	64.10	59.38	4.72
Ethylisobutylchlorosilane	39.21	43.88	-4.67
N,N-Dimethyl-N-ethylammonium acetate	33.05	37.62	-4.57
Bis(diethylamino)bis(dibutylamino)silane	130.21	134.71	-4.50
Dimethyldidecoxysilane	110.74	115.11	-4.37
Dimethyl decyl isopropylammonium bis(trifluoromethylsulfonyl)amide	111.11	106.76	4.35
Dixanthylene	114.20	109.92	4.28
Quadricyclane	30.01	25.75	4.26
Diethylammonium hydrogen sulfate	33.89	38.15	-4.26
Tetra-1-dodecoxysilane	233.40	237.66	-4.26
1-Benzyl-3-methylimidazolium 2-acryloamido-2-methylpropanesulfonate	103.89	99.64	4.25
Benzoylacetone	50.05	45.82	4.23
trans,trans-2,4-Hexadienoyl chloride	39.26	35.08	4.18
trans,trans-2,4-Heptadienal	38.87	34.70	4.17
Ethyl 3-methyl-3-phenylglycidate	59.88	55.74	4.14
9-H-Perfluorononyl 2-ethylhexanoate	90.16	86.05	4.11
1-(2-Cyanoethyl)-3-hexylimidazolium bis(2-ethylhexyl)sulfosuccinate	163.70	167.80	-4.10
Benzo[b]fluorene	76.21	72.11	4.10
1-Octyl-3-methylimidazolium thiocyanate	80.61	76.60	4.01
trans-Azobenzene	63.27	59.26	4.01
Fluoranthene	71.49	67.48	4.01

Vinylphenylphosphinic chloride	42.95	46.91	-3.96
1-Chloro-1,1-difluoroethane	20.31	16.36	3.95
1-Propyl-3-methylimidazolium methylsulfate	50.18	53.98	-3.80
Methyl ethylxanthate	34.82	38.54	-3.72
N,N-Dimethylaminotrimethylsilane	41.59	37.89	3.70
N-Hexylpyridinium trifluoroacetate	60.96	64.61	-3.65
3,3'-Dimethylazobenzene	72.51	68.88	3.63
Salicylic acid	31.18	34.80	-3.62
trans,trans-2,4-Hexadienal	33.64	30.07	3.57
2-Bromocyclohexanone	39.40	35.86	3.54
1-Phenyl-2-hexyl-3,5-dimethylpyrazolium tetrafluoroborate	85.60	82.07	3.53
Dipivaloylmethane	57.04	53.59	3.45
6,6,7,7,8,8,8-Heptafluoro-2,2-dimethyl-3,5-octanedione	53.47	50.03	3.44
N-Ethyl-N,N-dimethylammonium phenylacetate	58.89	62.20	-3.31
5-(Hydroxymethyl)-2-furaldehyde	33.94	30.63	3.31
Diethylammonium acetate	33.75	37.05	-3.30
Butyric aldehyde diethylacetal	45.68	42.39	3.29
Methylsuccinic acid	25.19	28.48	-3.29
Cinnamaldehyde	44.20	40.92	3.28
Tris(3-hydroxypropyl)phosphine	55.31	58.58	-3.27
Schradan	72.20	68.93	3.27
2,2'-Dimethylazobenzene	72.12	68.88	3.24
3-Ethylbenzoic acid	45.64	42.40	3.24
O,O,O-Triethyl thiophosphate	38.82	35.60	3.22
1-Nitro-2-phenoxybenzene	56.72	59.88	-3.16
3,4,5,6-Tetrahydro-7-methoxy-2H-azepine	39.49	36.35	3.14
2-Hydroxyethylammonium oleate	106.05	102.91	3.14
4-Nitrothioanisole	49.20	46.10	3.10
Ethyl fumarate	36.18	33.11	3.07
Benzylideneacetone	48.43	45.36	3.07
3-Methylbenzoyl chloride	44.67	41.64	3.03
2,2-Diethyl-1,3-propanediol	34.32	37.34	-3.02
Tri(1-phenylethoxy)borine	109.47	112.49	-3.02
Tetramethyldiaminobutane	49.95	47.00	2.95
1-Ethylthio-5,5-bis(ethoxy)-pent-1-en-3-yne	64.96	62.01	2.95
O,O-diisobutyl isobutylthiophosphinate	73.14	76.08	-2.94
(3-Bromo-1-propenyl)benzene	51.09	48.18	2.91
Octafluorobutyl-1,4-diisocyanate	38.69	35.80	2.89
Isopropyl phosphorusoxy dichloride	37.20	34.31	2.89
1,2-Dibromo-1,2-dichloroethane	39.24	36.36	2.88
Chloromethylsulfenyl chloride	23.73	26.61	-2.88
N'-Ethyl-N,N-dimethyl-1,2-ethanediamine	40.03	37.18	2.85
N-Isobutyl-3-sulfobutan-1-aminium hydrogen sulfate	64.42	67.27	-2.85
Phenylpropargyl aldehyde	42.36	39.52	2.84
Diethyl benzylidenemalonate	69.94	67.11	2.83
Pentafluorobenzenethiol	36.83	34.02	2.81
Oxotremorine	62.31	59.51	2.80
2-Methoxybenzylalcohol	42.09	39.30	2.79
3-(2-Cyanoethyl)-1-hexylimidazolium 3-sulfobenzoate	100.01	102.80	-2.79
4-t-Butylbenzoyl chloride	58.27	55.50	2.77
4-Phenyl-3-butyne-2-one	46.72	43.96	2.76
2-t-Butyl-5-methylphenol	54.59	51.84	2.75
Phenazine	59.11	56.36	2.75
4-Butylbenzoyl chloride	58.27	55.53	2.74
Ethyl 3-phenylpropionate	52.76	50.03	2.73
Cinnamionitrile	42.96	40.24	2.72
trans-Geranyl bromide	58.65	55.95	2.70
1,2-Bis(triethylsilyl)acetylene	79.93	82.62	-2.69
1-Butylthio-5,5-bis(ethoxy)-pent-1-en-3-yne	73.95	71.27	2.68
Cinnamic acid ethylester	54.30	51.62	2.68
Hydroxyacetaldehyde diethylacetal	37.22	34.55	2.67
Diethyl vinylphosphonate	39.62	42.28	-2.66
Hexamethylbenzene	52.72	55.38	-2.66
4-Pentylbenzoyl chloride	62.82	60.16	2.66
s-trans-Butadiene	22.69	20.04	2.65
2-Phenoxyvinyl diethoxy phosphorus oxide	71.10	68.45	2.65
1-Chloroanthracene	69.90	67.26	2.64
2,3-Dihydro-4H-1-benzopyran-4-one	43.36	40.72	2.64
2,6-Diethylaniline	52.09	49.45	2.64
1-Benzyl-3-(2-cyanoethyl)imidazolium thiocyanate	75.18	77.79	-2.61
Ethyl 2,4-dioxopentanoate	39.47	36.87	2.60
N-Ethylcarbazole	66.38	63.78	2.60
Methyl phenylpropionate	47.95	45.37	2.58
1,2-Dibromo-1,1-dichloroethane	39.24	36.67	2.57
2-Methoxyphenylisothiocyanate	50.47	47.90	2.57
1,1-Difluoroethane	13.83	11.28	2.55
Dicyclohexylphosphine	66.28	63.75	2.53

2-Methyl-3-phenyl-2-propenal	48.13	45.60	2.53
1,2,4-Triazole	17.50	14.98	2.52
Phenyl butoxy 2-(butoxycarbonyl)ethyl phosphorus oxide	86.28	88.79	-2.51
Cannabidiol	94.93	97.43	-2.50
Benz[a]anthracene	82.90	80.40	2.50
Tris(2-ethylhexyl) trimellitate	159.67	157.17	2.50
Vitamin K1	143.28	140.79	2.49
Cyclobutylol	51.72	49.23	2.49
Maleic anhydride	17.72	20.20	-2.48
Bis(2-hydroxyethyl)ammonium oleate	115.82	113.36	2.46
4-Tolunitrile	33.50	35.95	-2.45
Bis(diethylamino)bis(dipropylamino)silane	113.74	116.19	-2.45
7-H-Perfluoroheptyl methyl ether	46.04	43.61	2.43
4-nitrodiphenyl ether	62.31	59.88	2.43
1,3-Dioxolan-2-one	19.31	21.73	-2.42
Acetic acid 2-hydroxyethylester	26.22	23.80	2.42
trans-1,3,5-Hexatriene	31.55	29.14	2.41
Bis(trifluoroacetyl)methane	28.84	26.43	2.41
Triphenylphosphane	87.45	85.04	2.41
2-Methyl-5-isopropylaniline	47.00	49.40	-2.40
4-(1-Bromoethyl)-benzonitrile	50.76	48.36	2.40
1-Ethyl-3-methylimidazolium 2-acryloamido-2-methylpropanesulfonate	77.32	79.69	-2.37
Tri(butyl) ethylphosphonium diethylphosphate	105.37	107.73	-2.36
beta-Bromocinnamaldehyde	50.67	48.31	2.36
9H-Fluoren-9-one	56.81	54.45	2.36
Tetra-1-heptoxysilane	142.72	145.06	-2.34
Spiro(2,2)pentane	23.33	21.00	2.33
1-(2-Hydroxyethyl)-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	69.54	67.23	2.31
1,3,5-Tri-t-butylbenzene	80.22	82.53	-2.31
Phenyl butoxy 2-(butoxycarbonyl)propyl phosphorus oxide	91.07	93.37	-2.30
Diethyl oxobutanedioate	45.24	42.94	2.30
1,4-Diiodobenzene	49.38	51.68	-2.30
Phenyltrichlorosilylacetylene	58.54	56.24	2.30
Antimalarine	91.20	88.90	2.30
6-t-Butyl-2,4-dimethylphenol	58.94	56.65	2.29
4-Aminophenylacetate	44.17	41.88	2.29
Tetra(1H,1H,7H-perfluoroheptyl)silicate	149.98	152.26	-2.28
Trihexyl tetradecyl phosphonium acetate	173.57	171.29	2.28
Coronene	110.04	107.76	2.28
Potasan	85.31	83.05	2.26
(2-Methoxyvinyl)benzene	43.98	41.72	2.26
Hexadecanoic anhydride	154.37	152.12	2.25
1-(2-Hydroxyethyl)-3-methylimidazolium perfluorobutanesulfonate	63.29	65.53	-2.24
Chloropentafluorobenzene	33.07	30.84	2.23
Phenylisothiocyanate	43.58	41.35	2.23
2-Methylpropane	22.80	20.59	2.21
9-Methylanthracene	69.46	67.25	2.21
4-t-Butylbenzenemethanol	53.62	51.42	2.20
Bis-N-(2-hydroxypropyl)-2-furfurylamine	56.20	58.40	-2.20
Ethyl 2-benzylidene-2-cyanoacetate	53.73	55.92	-2.19
Methyl sorbate	38.11	35.92	2.19
N,N-Diisopropylethanolamine	46.50	44.32	2.18
Acetaldol	20.37	22.55	-2.18
1,3-Butadien-1-ol acetate	33.04	30.86	2.18
2-(Bromomethoxy)propane	29.09	31.27	-2.18
Bis(trihexyl)siloxane	189.57	187.40	2.17
9-Methyl-9H-fluorene	60.89	58.73	2.16
9-H-Perfluorononyl butyrate	69.74	67.58	2.16
5-Methoxy-2-methylindole	51.61	49.45	2.16
2-Butylthiovinyl dihexoxy phosphorus oxide	103.28	105.43	-2.15
1-Phenyl-2-pentyl-3,5-dimethylpyrazolium tetrafluoroborate	79.59	77.44	2.15
n-Undecanal	55.68	53.54	2.14
3-Acetyl-6-methylpyridine	41.08	38.94	2.14
4-Cyclohexylcyclohexyl acrylate	70.80	68.67	2.13
Hexachlorobenzene	53.31	55.44	-2.13
3-Cyclohexyl-2-methylnonane	71.81	73.93	-2.12
Triethyl-2-phenoxyethylsilane	72.79	74.91	-2.12
Ethyl sorbate	42.69	40.58	2.11
n-Butylstearate	103.61	105.72	-2.11
Ethyl trichloromethyl ether	34.31	32.21	2.10
Methyl 2-(methylamino)benzoate	48.76	46.66	2.10
4-t-Butyl-2,5-dimethylphenol	58.75	56.65	2.10
Cinnamoylchloride	48.03	45.93	2.10
1,4,5-Trimethyltetrahydro-8-naphthol	61.24	59.14	2.10
6-Nitro-9-oxaphenanthren-10-one	64.81	62.72	2.09

Tri-o-cresylphosphate	99.27	101.35	-2.08
2-Bromo-1,4-dimethoxybenzene	49.29	47.21	2.08
2-Fluoroethylsulfonyl fluoride	23.02	20.95	2.07
2-Oxobutyric acid	20.50	22.57	-2.07
3-(Phenylmethylene)-2-pentanone	56.73	54.67	2.06
2,6-Dimethylhepta-2,5-dien-4-one	45.92	43.87	2.05
1,4-Di-t-butylbenzene	61.81	63.86	-2.05
2-Acetylcyclopentanone	35.00	32.96	2.04
Benzamide	32.44	34.47	-2.03
cis-Cyclohexane-1,2-dinitrite	42.04	40.02	2.02
4-Methoxyphenyldipropylphosphine	73.12	71.11	2.01
S-Methyl thioacetate	26.05	24.04	2.01
Tri-sec-butoxymethane	69.40	67.40	2.00
4-Vinylaniline	41.71	39.71	2.00
Dibenzofuran	53.42	51.42	2.00
1-Aziridineethanol	21.77	23.76	-1.99
Benzenecarbothioic acid	37.13	39.11	-1.98
Monoacetin	27.89	29.85	-1.96
2,6-Di-t-pentyl-4-methylphenol	77.81	79.77	-1.96
N-Benzyl-N-ethylaniline	71.66	69.71	1.95
1-Bromo-4-t-butylbenzene	54.73	52.78	1.95
Methyl 3-bromopropanoate	32.04	30.10	1.94
Glycerol trioleate	268.81	270.75	-1.94
Forstab	100.03	98.09	1.94
Diphenylsulfone	62.21	60.27	1.94
2,3-Dimethylquinoxaline	47.17	49.10	-1.93
Pentafluorobenzonitrile	32.57	30.64	1.93
Isobutylphosphinic dichloride	37.98	39.91	-1.93
1-Butyl-3-methylimidazolium L-alanine	63.81	61.89	1.92
2,4-Dichloroaniline	38.29	40.21	-1.92
9,9'-Bifluorenyl	108.00	106.08	1.92
2-Fluorobenzeneacetoneitrile	37.59	35.67	1.92
N-Pentylpyridinium trifluoroacetate	58.06	59.98	-1.92
2-Phenoxyvinyl dimethoxy phosphorus oxide	61.05	59.13	1.92
Cinoxate	70.86	68.95	1.91
Cyclopropane	15.79	13.89	1.90
2-(Phenylmethylene)butanal	52.12	50.23	1.89
2-Fluorophenol	30.15	28.26	1.89
Bromoacetylene	18.64	16.76	1.88
1,4-Butanediamine	29.41	27.54	1.87
1-Cyano-1,3-butadiene	26.49	24.62	1.87
Dichloroethylmethylsilane	36.02	34.16	1.86
4-Hydroxybenzaldehyde	35.52	33.66	1.86
N-Methylmorpholinium formate	35.24	37.10	-1.86
EPN	86.83	84.97	1.86
Tartaric acid	24.89	26.74	-1.85
1,2-Diiodotetrafluoroethane	38.87	37.02	1.85
1-Butoxy-5,5-bis(ethoxy)-pent-1-en-3-yne	66.99	65.14	1.85
Tri-m-cresylphosphate	103.19	101.35	1.84
Perfluoroisoprene	25.97	24.13	1.84
1,3-Benzodioxole-5-ethanamine	43.73	45.56	-1.83
1,2-Dinitrobenzene	41.74	39.92	1.82
Perfluoro-n-octane	43.81	42.00	1.81
Tetradecoxysilane	198.82	200.62	-1.80
Benzylaniline	61.84	60.04	1.80
2-Isopropoxyvinyl diethoxy phosphorus oxide	59.43	57.63	1.80
cis-3-Phenyl-2-propenenitrile	42.03	40.24	1.79
Ethylcarbamate	22.59	20.81	1.78
N,N-Dimethyl-2-naphthylamine	60.34	58.56	1.78
1,3-Diphenyl-2-buten-1-one	71.77	69.99	1.78
Acetylacetone	27.65	25.87	1.78
Isobutylene	22.16	20.39	1.77
4,4'-Dibromodiphenyl ether	70.13	68.36	1.77
Bolecic acid	85.44	83.67	1.77
s-cis-Butadiene	21.80	20.04	1.76
s-trans-1,3-Butadiene	21.80	20.04	1.76
Hexyl ethoxy dithiophosphinic acid	63.48	65.23	-1.75
Ethyl 2-bromovalerate	45.80	44.05	1.75
2-Ethoxycarbonylaniline	48.13	46.38	1.75
trans-1,3-Butadienylbenzene	46.50	44.76	1.74
N,N-Diethyldodecanamide	81.75	80.01	1.74
9-Chloroanthracene	69.00	67.26	1.74
2-Vinyl-5-norbornene	40.67	38.94	1.73
3,4,5-Trimethoxybenzyl alcohol	50.67	52.40	-1.73
2-Ethoxyvinyl dimethoxy phosphorus oxide	45.41	43.68	1.73
4-Methoxybenzaldehyde	40.09	38.37	1.72
Ethoxyquin	69.39	67.68	1.71

4-Nitroaniline	35.57	37.27	-1.70
2-Phenylvinyl bis(dimethylamino) phosphorus oxide	71.90	70.20	1.70
Divinylacetylene	29.44	27.74	1.70
Nitroethylene	15.40	17.10	-1.70
9,10-Dihydrophenanthrene	60.48	58.78	1.70
N-(2-Hydroxyethyl)-bis(2-furfuryl)amine	58.60	60.30	-1.70
Tri(1,2-bis(ethoxycarbonyl)ethoxy)borine	130.83	132.53	-1.70
Dicyclohexylketone	56.58	58.27	-1.69
2,4,6-Cycloheptatrien-1-one	33.92	32.23	1.69
Tributylsilylaminotriethylsilane	104.73	106.42	-1.69
Dimethyldi(2-ethylhexoxy)silane	94.80	96.49	-1.69
4-Fluoroaniline	28.79	30.47	-1.68
1,2,3,5-Tetrafluorobenzene	27.80	26.12	1.68
Triphenylethylene	86.69	85.01	1.68
Hexanamide	34.71	33.04	1.67
2-Ethoxyvinyl diethoxy phosphorus oxide	54.67	53.00	1.67
Sulfuric acid	13.51	15.17	-1.66
sec-Butylstyrene	55.97	54.31	1.66
(-)-Globulol	67.93	66.28	1.65
Tetracyanoethylene	30.73	29.08	1.65
Stearic acid anhydride	172.28	170.64	1.64
N-Propylpyridinium trifluoroacetate	52.36	50.72	1.64
p-Anisylchloride	45.02	43.38	1.64
1-Methoxy-1,3-butadiene	27.74	26.10	1.64
2-Isopropoxyvinyl bis(diethylamino) phosphorus oxide	77.53	79.15	-1.62
Anethole	48.60	46.98	1.62
Saccharose	67.70	69.32	-1.62
Sanger's Reagent	41.43	39.82	1.61
Octafluoroanisole	33.75	32.14	1.61
Dimethyldi-2-heptoxysilane	85.72	87.33	-1.61
1-(2-Phenylethoxy)-5,5-bis(ethoxy)-pent-1-en-3-yne	82.06	80.46	1.60
1,2,3,4,5,6,7,8-Octahydrophenanthrene	58.44	60.04	-1.60
beta-Ionone	61.84	60.24	1.60
N-(2-Hydroxypropyl)-bis(2-furfuryl)amine	63.34	64.93	-1.59
iso-Pentyl 4-methylpentoxy dithiophosphinic acid	80.61	79.02	1.59
2-Nitrobenzeneethanol	45.67	44.08	1.59
Triethylene glycol dimethacrylate	71.75	73.34	-1.59
Propyldichlorophosphine	33.74	35.33	-1.59
6,6-Dimethylfulvene	38.24	36.66	1.58
4-t-Amylstyrene	60.53	58.96	1.57
trans-(3-Chloro-1-propenyl)benzene	46.82	45.25	1.57
Tripropylsilanol	55.59	54.03	1.56
N,N-Dimethyl-2-nitroaniline	48.86	47.30	1.56
1,3-Divinylbenzene	46.36	44.80	1.56
Propyne	15.51	13.96	1.55
Quinine	93.86	95.40	-1.54
2-Acetylcyclohexanone	39.13	37.59	1.54
N,N-Diethyl-2-methylaniline	53.04	54.57	-1.53
Ethyl 4,4,4-trifluoroacetoacetate	33.75	32.22	1.53
Bis(trifluoroacetyl)methane (enol form)	28.84	27.31	1.53
Diheptyl terephthalate	105.99	104.46	1.53
trans-2-Butenedinitrile	21.63	20.10	1.53
2-Phenoxypropionic acid	42.47	43.99	-1.52
Benzenesulfinylchloride	39.52	41.04	-1.52
(Ethoxy fluoro oxophosphorus) (bis(diethylamino) oxophosphorus) oxide	74.30	72.78	1.52
4-(4-Bromophenoxy)toluene	67.10	65.58	1.52
1-Methoxy-4-trifluoromethoxy-2,3,5,6-tetrafluorobenzene	40.30	38.79	1.51
Acetylisothiocyanate	26.81	25.30	1.51
2-Methyl-7,8-benzoquinoline	63.25	64.75	-1.50
2,5-Norbornadiene	28.37	29.87	-1.50
2-Nitro-m-xylene	41.34	42.84	-1.50
1-Pent-4-enylphosphine	33.47	34.97	-1.50
1,2-Dimethyl-4-nitrobenzene	41.34	42.84	-1.50
2-Isopropoxyvinyl dimethoxy phosphorus oxide	49.81	48.31	1.50
3,5-Diethoxy-5-methylhexanal	49.07	47.57	1.50
trans,cis-2,4-Hexadiene	31.08	29.58	1.50
Glycerol trinitrate	40.39	38.90	1.49
N-(2-Furfuryl)thiomorpholine	50.61	52.10	-1.49
1-Ethyl-5-methylpyrazole	31.53	33.02	-1.49
Ethyl cyclohexanecarboxylate	44.85	43.36	1.49
2-Isobutenylfuran	39.06	37.57	1.49
1-Fluoro-3-isothiocyanatobenzene	42.29	40.80	1.49
Ethoxyacetylene	22.08	20.59	1.49
2,N,N-Trimethylaniline	43.92	45.41	-1.49
2,N,N-Trimethylaniline	43.92	45.41	-1.49
N-Hexylpyridinium bis(trifluoromethanesulfonyl) amide	84.06	85.55	-1.49

1-Benzyl-3-methylimidazolium chloride	58.45	59.94	-1.49
L-Proline 2-methylpropyl ester dodecyl sulfate	116.75	115.26	1.49
Chloromethyldiphenylsilane	68.14	69.62	-1.48
L-Valine 2-methylpropyl ester dodecyl sulfate	118.59	117.11	1.48
Propyl 4-hydroxybenzoate	50.28	48.80	1.48
Benzylazide	38.58	40.06	-1.48
cis-Stilbene	61.86	60.38	1.48
1-Methoxy-1-buten-3-yne	25.83	24.35	1.48
1,1,2,2-Tetrafluoroethoxycyclohexane	40.68	39.20	1.48
Cyclooctanamine	38.98	40.45	-1.47
alpha-Farnesene	69.47	70.94	-1.47
1,3-Dihydroxybenzene	28.74	30.20	-1.46
1-(1-Methyl-1H-pyrrol-2-yl)ethanone	37.01	35.55	1.46
4-Acetylphenol	39.56	38.10	1.46
1-Benzyl-3-methylimidazolium methylsulfate	67.84	69.30	-1.46
Methyltripropoxysilane	61.92	60.47	1.45
1,2-Divinylbenzene	46.25	44.80	1.45
2-Phenyl-2-propanol	43.39	41.94	1.45
4-Bromoaniline	36.71	38.16	-1.45
Bis(dimethylamino)borane	31.63	33.07	-1.44
4-Methyl-1,3-pentadiene	30.93	29.49	1.44
1-Vinyl-4-methoxybenzene	43.65	42.21	1.44
1-Vinyl-3-methoxybenzene	43.65	42.21	1.44
Coumatetralyl	84.30	82.86	1.44
Butyl oleate	104.13	105.56	-1.43
Bromomethylacetate	25.24	26.67	-1.43
1-Allyl-3-(2-cyanoethyl)imidazolium thiocyanate	60.96	62.39	-1.43
Methyl trioctylammonium bis(trifluoromethylsulfonyl)amide	154.51	153.08	1.43
Isoheptyl methoxy dithiophosphinic acid	63.84	65.26	-1.42
4,4-Diethoxy-1-butanamine	44.42	45.84	-1.42
trans-Piperylene	26.23	24.81	1.42
2,3'-Bipyridine	48.27	46.85	1.42
trans-2-Methoxy-4-(1-propenyl)phenol	50.24	48.82	1.42
Dichloroacetylene	19.36	20.78	-1.42
Methyl 2-aminobenzoate	43.13	41.72	1.41
2-(1-Pentenyl)furan	43.70	42.29	1.41
Cumulene	17.25	15.84	1.41
1-Butyne	20.00	18.59	1.41
Methylparathion	60.50	61.91	-1.41
9-Bromoanthracene	71.44	70.03	1.41
Octadecanenitrile	83.86	85.27	-1.41
1,5-Dimethylpyrazole	27.04	28.44	-1.40
N-Methyl-p-toluidine	41.72	40.32	1.40
Tritetralin	75.40	76.80	-1.40
Phenylphosphonic dichloride	45.88	44.49	1.39
Tetrabutylphosphonium butyrate	105.08	106.47	-1.39
2-Hydroxypropylmethacrylate	36.05	37.44	-1.39
Isosafrol	47.97	46.58	1.39
1-Hexadecanol	76.24	77.62	-1.38
3-Chloronitrobenzene	36.66	38.04	-1.38
1,2-Diphenylethane	59.16	60.54	-1.38
Biphenyl	49.90	51.28	-1.38
1,2-Diiodoethane	38.54	37.16	1.38
Diethylmethyl 1-isobutoxyethoxysilane	66.14	64.76	1.38
Diethyleneglycol dimethacrylate	60.99	62.37	-1.38
1,2-Dimethoxy-4-(1-propenyl)benzene	54.91	53.53	1.38
1-(Chloromethyl)-4-methoxybenzene	41.33	42.70	-1.37
Panthenol	50.05	51.42	-1.37
1,10-Dibromodecane	65.29	63.92	1.37
N,N-Diethylcarbamic acid	32.00	30.63	1.37
Julolidine	56.51	55.14	1.37
Methyldichloroisobutoxysilane	43.20	44.57	-1.37
Diphenylsulfoxide	61.40	60.04	1.36
Diethyl acetylenedicarboxylate	42.44	41.08	1.36
Dimethyl pimelate	45.85	47.21	-1.36
Quinoxaline	40.50	39.14	1.36
4-Methoxy-1,1'-biphenyl	59.18	57.83	1.35
1-n-Propylimidazole	31.28	32.63	-1.35
2-Phenylfuran	45.05	43.70	1.35
Tridecanoic acid	65.28	63.94	1.34
1-(2-Hydroxyethyl)-3-(2-cyanoethyl)imidazolium thiocyanate	60.35	59.01	1.34
1-Chloro-2-methyl-1-butene	28.50	29.84	-1.34
5-Methylfurfural	30.55	29.21	1.34
4-Methylpentyl ethoxy dithiophosphinic acid	63.85	65.18	-1.33
2-(Vinylloxy)ethanol	24.41	23.08	1.33
2-Iodobiphenyl	65.19	63.86	1.33
trans-1-Propenylbenzene	41.76	40.43	1.33

2,3,4,5-Tetramethylpyrrole	41.21	39.88	1.33
Tetra(2,2-diethylhydrazino)silane	114.23	112.91	1.32
sec-Hexyl acetate	39.53	40.85	-1.32
cis-1,3,5-Hexatriene	30.46	29.14	1.32
Isopropenylacetylene	24.29	22.97	1.32
Dichloro(4-ethylphenyl)phosphine	56.02	54.70	1.32
Phenethyl acetate	45.65	46.96	-1.31
Ethylphenylsilanol	47.88	46.57	1.31
3-Methyl-1,3-butanediol	29.35	28.04	1.31
beta-Irone	66.08	64.77	1.31
Isoindole	38.60	37.29	1.31
1-Ethyl-3-methylimidazolium hydrogen sulfate	44.57	45.88	-1.31
1,2-Dichloro-1-ethoxyethane	33.38	32.08	1.30
1,6-Hexanedial	29.70	31.00	-1.30
2-Ethylpyrrole	31.77	30.47	1.30
1,3,5-Tris(3-methoxypropyl)borazine	83.61	84.90	-1.29
3,5-Dichloroaniline	41.50	40.21	1.29
3-Methylbutanoic anhydride	48.87	50.16	-1.29
Ethyl N,N-diethylamino phosphorusoxy fluoride	41.53	40.24	1.29
Acetoacetic acid ethylester Enolform	34.11	32.82	1.29
Phenothrin	104.96	103.67	1.29
1-(2-Cyanoethyl)-3-octylimidazolium bis(2-ethylhexyl)sulfosuccinate	175.77	177.06	-1.29
Tricyclene	40.57	41.85	-1.28
Isobornyl thiocynoacetate	66.31	67.59	-1.28
p-Isopropenylstyrene	50.76	49.48	1.28
1,2-Dihydroxybenzene	31.48	30.2	1.28
cis,cis-2,4-Hexadiene	30.86	29.58	1.28
1-Vinylnaphthalene	52.40	53.68	-1.28
Butylisobutylether	42.08	40.80	1.28
Ethyl benzoylacetate	53.15	51.87	1.28
1,1-Dichlorotetrafluoroethane	22.58	21.30	1.28
5-Methyl-1-phenyl-1-hexen-3-one	60.48	59.20	1.28
Glycerol tripalmitate	242.2	243.47	-1.27
Aramite	87.62	86.35	1.27
1,1-Diphenyl-1-propene	63.79	65.06	-1.27
2,5-Dimethyl-2,4-hexadiene	40.21	38.94	1.27
2-Phenylpyridine	50.39	49.12	1.27
4-Methoxyacetophenone	44.02	42.75	1.27
1,1,1,2,2,3,3-Heptafluorobutane	22.95	21.68	1.27
Furoylchloride	30.50	29.23	1.27
Naphthalene	43.21	44.48	-1.27
1,5-Cyclooctadiene	35.45	36.72	-1.27
Tetra-2-ethyl-1-hexoxysilane	162.11	163.38	-1.27
Fluorosulfonylbenzene	35.05	36.31	-1.26
9-Heptyl-9-heptadecanol	113.35	114.61	-1.26
N,N-Dimethyltrichloroacetamide	40.42	39.16	1.26
cis-1,3-Hexadiene	30.66	29.40	1.26
N-Ethyl-3-methylaniline	46.16	44.90	1.26
4-Mercaptophenol	35.10	36.36	-1.26
1,2-Dichlorotetrafluoroethane	22.58	21.32	1.26
Paraoxon	64.85	63.60	1.25
2-Hydroxybenzoyl chloride	39.81	38.57	1.24
Phenylhydrazine	34.06	not evaluable	
Malathion	77.17	not evaluable	
N-(Diethylaminothiocarbonyl)-N',N'-diethylbenzamidine	91.29	not evaluable	
2-Pyrazoline	19.51	not evaluable	
Chlorotrifluoroethylene	17.52	not evaluable	
1-Butyl-3-methylimidazolium iodide	58.90	not evaluable	
1-Hexyl-3-methylimidazolium iodide	67.74	not evaluable	