

Electronic supporting information for *Predicting Melting Points of Organic Molecules: Applications to Aqueous Solubility Prediction Using the General Solubility Equation.*

Table S1. The chemical names, logP from AlogP and melting point in degrees Celsius of the molecules in dataset MP1100.

Chemical Name	logP (AlogP)	Melting Point (°C)
(1,2-dibromoethyl)benzene	4.01	72
(1-bromoethyl)benzene	3.61	-65
(1R)-camphor	2.85	177.5
(1R)-camphor-10-sulfonic acid	-0.53	200
(1R)-camphor-10-sulfonyl chloride	2.06	66
(1R)-camphorquinone	2.57	199.5
(1R)-endo-fenchyl alcohol	2.3	40.5
(1R,2s)-10,2-camphorsultam	1	180.5
(1R,3S)-camphoric acid	1.51	185.5
(1S)-camphanic acid	1.77	200
(1S)-camphanic chloride	2.15	66
(1S)-camphor	2.85	177.5
(1S)-camphor-10-sulfonyl chloride	2.06	66
(1S)-camphorquinone	2.57	198.5
(1S)-camphorsulfonylimine	1.55	227
(1S,2R)-10,2-camphorsultam	1	183
(1S,2R)-1-phenyl-2-(1-pyrrolidinyl)-1-propanol	2.04	45
(1S,4S)-2-boc-2,5-diazabicyclo(2.2.1)heptane	0.72	75
(2-aminoethoxy)acetic acid	-3.18	178
(2-bromoethyl)benzene	3.28	-56
(2-carboxyphenyl)iminodiacetic acid	0.81	217
(2h)1,4-benzothiazin-3(4h)-one	1.65	177
(2-hydroxyethyl)hydrazine	-1.48	-70
(2S,5s)-2,5-hexanediol	0.31	53
(3,4-dimethoxyphenylthio)acetic acid	2	102
(3-bromo-2,4,6-trimethylphenylcarbamoyl)methyliminodiacetic acid	-0.39	194
(3-chloropropyl)trimethoxysilane	1.98	-50
(3R-cis)-tetrahydro-3-trichloromethyl-1h,3h-pyrrolo(1,2-c)oxazol-1-one	2.06	110
(3S,4R)-4-(4-fluorophenyl)-1-methyl-3-piperidinemethanol	2.06	95.5
(4-bromobutoxy)benzene	3.73	41.5
(4-chlorophenoxy)acetyl chloride	2.65	19
(4-chlorophenylsulfonyl)acetonitrile	1	171
(4-chlorophenylthio)acetic acid	2.71	105.5
(4-chlorophenylthio)acetonitrile	2.91	80
(4-fluorophenylthio)acetic acid	2.05	77.5
(4-fluorophenylthio)acetonitrile	2.31	33.5
(4-imidazolyl)acetonitrile	0.43	137
(4-tert-butylphenoxy)acetonitrile	3.37	68.5

(5-mercapto-1,3,4-thiadiazol-2-ylthio)acetic acid	0.31	167
(benzylthio)acetic acid	2.2	61.5
(chloromethyl)cyclopropane	2.12	-91
(e)-3-dimethylamino-1-(2-pyridyl)-2-propen-1-one	0.49	131
(e)-alpha-(4-chlorophenyl)cinnamionitrile	4.44	115.5
(e)-alpha-methylstilbene	4.84	80.5
(methoxymethyl)diphenylphosphine oxide	1.63	117
(methylamino)acetaldehyde dimethyl acetal	-0.3	-73
(methylthio)acetic acid	-0.15	13.5
(pentafluorophenyl)diphenylphosphine	5.02	71
(phenylsulfonyl)acetamide	-0.36	156
(phenylsulfonyl)acetic acid	0.18	111.5
(phenylthio)acetic acid	2.28	63.5
(R)-1-boc-3-hydroxypiperidine	1.51	46.5
(R)-3-(boc-amino)-3-(4-bromophenyl)propionic acid	3.01	144
(R)-3-boc-thiazolidine-2-carboxylic acid	1.15	91.5
(R)-limonene	4.5	-74
(S)-1-boc-3-hydroxypiperidine	1.51	37
(S)-2-(6-methoxy-2-naphthyl)propionic acid	3.29	155
(S)-2-(boc-amino)-4-phenylbutyric acid	2.92	78
(S)-2-pyrrolidinone-5-carboxylic acid	-1.01	160
(S)-3-(boc-amino)-4-(4-pyridyl)butyric acid	1.43	141.5
(S)-3-(boc-amino)-4-phenylbutyric acid	2.82	104
(S)-3-(boc-amino)-5-methylhexanoic acid	2.23	54
(S)-3-(boc-amino)piperidine	1.17	124.5
(S)-3-boc-thiazolidine-2-carboxylic acid	1.15	91.5
(S)-4-sec-butyloxazolidine-2,5-dione	0.73	65.5
(S)-alpha-methoxy-alpha-(trifluoromethyl)phenylacetic acid	2.01	44
(S)-nicotine	0.87	-79
(S,s)-hydrobenzoin	2.05	149
(trimethylsilyl)acetic acid	1.33	41
(2.2)paracyclophane	5.23	285.5
(4-(trifluoromethyl)phenylsulfonyl)acetonitrile	1.49	143.5
(4-(trifluoromethyl)phenylthio)acetic acid	2.98	116
1-(1-methyl-4-piperidinyl)piperazine	0.1	30.5
1-(1-propynyl)cyclohexanol	2.49	48
1-(2,4,6-triisopropylphenylsulfonyl)-1,2,4-triazole	3.03	111
1-(2,4-difluorophenyl)piperazine	1.43	75
1-(2,5-dimethylphenyl)piperazine	2.18	44.5
1-(2-aminoethyl)piperazine	-1.4	-19
1-(2-aminophenyl)pyrrole	2.06	93.5
1-(2-bromoethyl)-4-nitrobenzene	3.12	69
1-(2-fluorophenyl)piperazine	1.35	46
1-(2-furoyl)piperazine	-0.13	68
1-(2-furyl)-2-nitroethylene	1.39	73.5
1-(2-hydroxyethyl)-2-imidazolidinone	-1.57	48.5

1-(2-hydroxyethyl)piperazine	-1.67	-39
1-(2-hydroxyethyl)piperidine	0.56	16
1-(2-methoxyethyl)homopiperazine	-0.26	66.5
1-(2-methoxyphenyl)piperazine	1.42	37
1-(2-naphthoyl)-3,3,3-trifluoroacetone	3.29	74
1-(2-naphthyl)ethanol	2.77	73.5
1-(2-nitrophenyl)piperidine	3.29	77
1-(2-nitrophenyl)pyrrole	2.81	59
1-(2-phenylethyl)-4-(phenylethynyl)benzene	6.07	105
1-(2-phenylethyl)-4-piperidone	1.81	58
1-(2-pyridylazo)-2-naphthol	3.87	139.5
1-(2-thenoyl)-3,3,3-trifluoroacetone	2.37	42.5
1-(2-thiazolylazo)-2-naphthol	4.17	139
1-(2-trifluoromethylphenyl)imidazole	2.28	51.5
1-(3,4-dichlorophenyl)piperazine	2.72	63
1-(3,4-dimethylphenyl)piperazine	2.18	62.5
1-(3,5-dichlorophenyl)-2,5-dimethyl-1h-pyrrole	4.83	79
1-(3-aminophenyl)ethanol	0.49	67.5
1-(3-aminopropyl)imidazole	-0.71	-68
1-(3-chlorophenoxy)-3-butyn-2-ol	2.04	38
1-(3-hydroxypropyl)piperazine	-1.22	50
1-(3-methoxybenzoyl)-2-(1-naphthoyl)hydrazine	2.83	190
1-(3-trifluoromethylphenoxy)-3-butyn-2-ol	1.87	31.5
1-(4-aminophenyl)ethanol	0.5	69.5
1-(4-biphenyl)ethanol	3.42	97
1-(4-bromophenyl)ethanol	2.45	37
1-(4-chlorophenyl)cyclohexane-1-carboxylic acid	3.73	152
1-(4-chlorophenyl)cyclopropanecarboxylic acid	2.76	153.5
1-(4-chlorophenylsulfonyl)-3,3-dimethyl-2-butanone	2.69	97
1-(4-ethoxyphenyl)ethanol	2.28	46.5
1-(4-ethoxyphenyl)ethynyl-4-n-pentylbenzene	6.42	62
1-(4-fluorophenyl)piperazine	1.49	31.5
1-(4-fluorophenyl)pyrrole	2.77	51
1-(4-hydroxyphenyl)-5-mercaptotetrazole	1.31	170
1-(4-iodophenyl)pyrrole	3.57	130.5
1-(4-methoxy-4-biphenylsulfonyl)proline	2.18	154
1-(4-methoxybenzoyl)-2-(1-naphthoyl)hydrazine	2.86	188.5
1-(4-methoxyphenyl)-1-cyclohexanecarbonitrile	3.81	43
1-(4-methoxyphenyl)-1h-1,2,4-triazole	1.16	97
1-(4-methoxyphenyl)ethynyl-4-n-pentylbenzene	6.13	47
1-(4-methoxyphenyl)ethynyl-4-n-propylbenzene	5.3	61
1-(4-methoxyphenyl)imidazole	1.62	66
1-(4-nitrophenyl)-3-(2-thienyl)-2-propen-1-one	3.53	169
1-(4-nitrophenyl)-5-(trifluoromethyl)-1h-pyrazole-4-carboxylic acid	2.68	201
1-(4-nitrophenyl)glycerol	0.74	96
1-(4-nitrophenyl)piperazine	1.27	131

1-(4-nitrophenyl)piperidine	3.37	103.5
1-(4-nitrophenylazo)-2-naphthol	5.04	250
1-(4-pyridyl)piperazine	0.56	138.5
1-(6-methoxy-2-naphthyl)ethanol	2.9	111.5
1-(boc-amino)cyclopentanecarboxylic acid	2.12	132.5
1-(chloromethyl)naphthalene	3.91	32
1-(cyanoacetyl)piperidine	0.49	87.5
1-(cyanoacetyl)pyrrolidine	-0.14	72.5
1-(heptafluorobutyryl)imidazole	2.4	10.5
1-(methylsulfonyl)imidazole	-1.01	88.5
1-(o-tolyl)piperazine	1.7	46.5
1-(pentafluorobenzoyl)imidazole	2.51	55.5
1-(pentafluorophenyl)ethanol	1.94	33
1-(phenylethynyl)cyclohexanol	3.34	61
1-(phenylsulfonyl)indole	2.56	78
1-(phenylsulfonyl)pyrrole	1.53	88.5
1-(p-toluenesulfonyl)indole	2.73	85
1-(p-toluenesulfonyl)pyrrole	1.66	101
1-(trans-cinnamoyl)imidazole	2.14	130
1-(trifluoromethyl)cyclohexanecarboxylic acid	1.71	69.5
1-(trifluoromethyl)cyclopentanecarboxylic acid	1.39	37
1-(trimethylsilyl)imidazole	0.78	-42
1,1-(azodicarbonyl)dipiperidine	2.09	134.5
1,1,1,2-tetrafluoro-2-iodo-2-(trifluoromethoxy)ethane	2.55	43.5
1,1,1,3,3,3-hexafluoro-2-propanol	2.58	-3
1,1,1-tris(chloromethyl)ethane	2.86	18
1,1,1-tris(hydroxymethyl)ethane	-1.34	190
1,1,2,2-tetrachloroethane	2.57	-43
1,1,2,2-tetrafluoroethyl methyl ether	1.83	-107
1,1,2-trichloro-3,3,3-trifluoro-1-propene	3.19	-114
1,1,2-trimethyl-1h-benzo(e)indole	4.38	116.5
1,1,3,3,5,5-hexamethyltrisiloxane	2.71	-67
1,1,3,3-tetramethyldisiloxane	1.66	-78
1,1,3-triphenylpropargyl alcohol	4.6	81
1,1,4,4-tetraphenyl-1,3-butadiene	7.24	197.5
1,1:3,1-terphenyl-5-boronic acid	4.34	294
1,10-decanedicarbonitrile	2.86	17.5
1,10-decanediol	2.7	72.5
1,10-decanedithiol	4.77	17
1,10-dibromodecane	3.6	28
1,10-diiododecane	5.55	30
1,10-phenanthroline, anhydrous	2.31	117.5
1,12-diaminododecane	3.47	70
1,12-dibromododecane	5.61	40
1,12-dodecanediol	3.74	82.5
1,18-octadecanedicarboxylic acid	6.79	127

1,1-bi(2-naphthol)	4.6	216.5
1,1-bis(methylthio)-2-nitroethylene	0.87	125.5
1,1-carbonyldiimidazole	-0.33	118
1,1-carbonyldipiperidine	1.61	44.5
1,1-cyclohexanediactic acid	1.31	180
1,1-cyclopropanedicarboxylic acid	-0.21	131.5
1,1-cyclopropanedicarboxylic acid monomethyl ester	0.28	49
1,1-dioxobenzo(b)thiophen-2-ylmethyl chloroformate	1.69	76.5
1,1-diphenyl-2-propyn-1-ol	3.04	46
1,1-diphenylacetone	3.57	61
1,1-diphenylethanol	3.3	80
1,1-diphenylethylene	4.53	6
1,1-thiocarbonyldi-2(1h)-pyridone	1.59	164.5
1,2,3,4-tetrafluorobenzene	2.34	-42
1,2,3,4-tetrahydrocarbazole	3.77	119
1,2,3,4-tetrahydroisoquinoline	1.31	-30
1,2,3,4-tetrahydronaphthalene	3.79	-36
1,2,3,4-tetrahydroquinoline	2.27	14
1,2,3-benzotriazin-4(3h)one	0.25	223
1,2,3-hexanetriol	-0.85	65.5
1,2,3-thiadiazole-4-carboxaldehyde	0.25	85
1,2,3-thiadiazole-4-carboxylic acid	-0.66	227.5
1,2,3-triacetoxybenzene	1.58	166
1,2,3-tribromopropane	3.24	16.5
1,2,3-trichloro-4-nitrobenzene	3.65	54.5
1,2,3-trichloro-5-nitrobenzene	3.69	69.5
1,2,3-trichlorobenzene	4.07	54
1,2,3-trichloropropane	2.29	-14
1,2,3-trimethoxybenzene	2.02	44
1,2,4,5-tetrabromobenzene	5.03	177.5
1,2,4,5-tetrachlorobenzene	4.61	140
1,2,4,5-tetrafluorobenzene	2.43	4
1,2,4,5-tetrakis(isopropylthio)benzene	7.01	77
1,2,4,5-tetramethylbenzene	4.05	78.5
1,2,4-benzenetricarboxylic anhydride	0.98	167
1,2,4-butanetriol	-1.59	-20
1,2,4-triacetoxybenzene	1.63	99
1,2,4-triazole	-0.8	120
1,2,4-triazolo(4,3-a)pyridin-3(2h)-one	0.19	234
1,2,4-triazolo(4,3-a)pyridine-3-thiol	1.2	209.5
1,2,4-tribromobenzene	4.42	42
1,2,4-trichloro-5-iodobenzene	4.48	103.5
1,2,4-trichlorobenzene	4.08	17
1,2,4-trifluoro-5-nitrobenzene	1.97	-11
1,2,4-trimethylbenzene	3.62	-44
1,2,4-triphenyl-1,4-butanedione	4.81	128

1,2,5-trichloro-3-iodobenzene	4.47	52
1,2,6-hexanetriol	-0.8	-20
1,2-benzenedimethanol	0.33	61.5
1,2-benzenedithiol	1.8	23
1,2-benzisoxazol-3(2h)-one	0.79	138.5
1,2-bis(1-naphthyl)ethane	6.63	161.5
1,2-bis(2-chloroethoxy)ethane	1.26	-32
1,2-bis(2-nitrophenoxy)ethane	3.29	168.5
1,2-bis(carboxymethylthio)ethane	0.11	110
1,2-bis(chlorodimethylsilyl)ethane	3.58	37
1,2-bis(dimethoxyphosphoryl)benzene	0.78	81
1,2-bis(dimethylphosphino)ethane	2.77	179.5
1,2-bis(diphenylphosphino)benzene	7.92	187
1,2-bis(diphenylphosphino)ethane	6.88	140.5
1,2-bis(methanesulfonamido)benzene	0.14	212.5
1,2-bis(phenylsulfonyl)ethane	1.6	179.5
1,2-bis(phenylthio)ethane	4.98	69
1,2-bis(2-(trifluoromethyl)phenyl)ethane	5.19	75
1,2-cyclohexanedione	0.77	36.5
1,2-di(3-indenyl)ethane	5.88	123
1,2-di(p-tolyl)ethane	5.79	81
1,2-diaminopropane	-1.36	-37
1,2-dianilinoethane	3.34	66
1,2-dibenzoylbenzene	4.51	146.5
1,2-dibenzoylethane	3.2	146
1,2-dibromo-2,4-dicyanobutane	2.14	50
1,2-dibromo-3,5-difluorobenzene	3.62	37
1,2-dibromo-4,5-difluorobenzene	3.67	33
1,2-dibromobenzene	3.77	5
1,2-dibromobutane	3.38	-65
1,2-dibromoethane	2.08	9.5
1,2-dibromopropane	2.65	-55
1,2-dichloro-3-iodobenzene	4.07	35
1,2-dichloro-3-nitrobenzene	3.05	62
1,2-dichloro-4-fluorobenzene	3.46	-1
1,2-dichloro-4-iodobenzene	4.07	30
1,2-dichloro-4-nitrobenzene	3.11	41
1,2-dichlorobenzene	3.45	-18
1,2-dichloroethane	1.48	-35
1,2-dichloropropane	2.13	-100
1,2-diethoxybenzene	3.09	44
1,2-diethoxyethane	0.78	-74
1,2-diethylbenzene	4.55	-31
1,2-difluoro-4,5-dimethoxybenzene	2.2	40
1,2-difluorobenzene	2.24	-34
1,2-dihydronaphthalene	3.53	-8

1,2-diiodoethane	2.72	82
1,2-dimethoxy-4,5-dinitrobenzene	1.58	132.5
1,2-dimethoxyethane	0.03	-69
1,2-dimethyl-5-nitroimidazole	-0.01	137
1,2-dimethylimidazole	0.37	36.5
1,2-diphenoxyethane	3.42	95
1,2-diphenylethane	4.74	51.5
1,2-epoxyoctadecane	8.31	32.5
1,2-ethanedithiol	0.84	-41
1,2-ethylenediphosphonic acid	-0.89	219
1,2-octanediol	1.66	31
1,2-o-isopropylidene-alpha-D-glucofuranose	-0.94	159.5
1,2-phenylene phosphorochloridite	2.53	30
1,2-phenylenediacetic acid	1.2	151
1,2-phenylenediacetonitrile	0.69	59
1,2-propanediol	-1.1	-60
1,2-propanediol diacetate	0.77	-31
1,3,3-trimethyl-2-methyleneindoline	3.38	-10
1,3,5,7-cyclooctatetraene	3.1	-5
1,3,5-benzenetricarbonyl chloride	3.12	36
1,3,5-benzenetricarboxylic acid	0.87	375
1,3,5-tribenzoylbenzene	5.45	117.5
1,3,5-tribenzylhexahydro-1,3,5-triazine	3.42	50
1,3,5-tribromobenzene	4.42	122.5
1,3,5-trichloro-2,4,6-trifluorobenzene	4.06	63
1,3,5-trichloro-2-iodobenzene	4.48	54.5
1,3,5-trichloro-2-nitrobenzene	3.6	70.5
1,3,5-trichlorobenzene	4.08	63.5
1,3,5-triethynylbenzene	2.03	106
1,3,5-trifluoro-2-nitrobenzene	1.89	3.5
1,3,5-trifluorobenzene	2.36	-5.5
1,3,5-triisopropylbenzene	5.52	-7
1,3,5-trimethoxy-2-nitrobenzene	1.65	151.5
1,3,5-trimethoxybenzene	1.96	52
1,3,5-trimethyl-1h-pyrazole	0.73	35.5
1,3,5-trimethyl-1h-pyrazole-4-carboxaldehyde	0.58	81.5
1,3,5-trioxane	-0.95	60.5
1,3,5-triphenylbenzene	7.3	173
1,3,5-tris(2-hydroxyethyl)cyanuric acid	-1.57	138
1,3,5-tri-tert-butylbenzene	7.17	71
1,3-benzenedimethanol	0.28	58
1,3-benzenedisulfonyl chloride	1.66	59
1,3-benzodioxole	1.71	-18
1,3-bis(2-hydroxyhexafluoroisopropyl)benzene	3.66	9.5
1,3-bis(4-piperidiny)propane	2.73	65.5
1,3-bis(diphenylphosphino)propane	7.23	60.5

1,3-bis(hydroxymethyl)urea	-2.19	126
1,3-bis(trifluoromethyl)benzene	3.7	-35
1,3-bis((trimethylsilyl)ethynyl)benzene	4.73	58
1,3-bis(tris(hydroxymethyl)methylamino)propane	-2.14	169
1,3-cyclohexadiene	2.3	-89
1,3-cyclohexanediol, cis trans	0.02	30
1,3-cyclohexanedione	0.34	103
1,3-cyclooctadiene	3.56	-53
1,3-cyclopentanedione	-0.14	152
1,3-di(4-pyridyl)propane	2.39	54.5
1,3-di-2-thienyl-2-propen-1-one	3.6	99
1,3-diacetylbenzene	1.68	36
1,3-diacetylimidole	2.29	145.5
1,3-diamino-2-propanol	-1.99	42.5
1,3-diaminopropane	-1.41	-12
1,3-dibenzoylbenzene	4.6	98.5
1,3-dibenzoyloxybenzene	4.42	117.5
1,3-dibenzyl-5-cyanohexahydropyrimidine	2.62	79.5
1,3-dibromo-2,2-diethylpropane	4.39	39.5
1,3-dibromo-2,2-dimethoxypropane	1.88	65.5
1,3-dibromo-5-fluoro-2-iodobenzene	4.08	134
1,3-dibromobenzene	3.73	-7
1,3-dibromopropane	2.55	-34
1,3-dichloro-2-fluorobenzene	3.48	38
1,3-dichloro-2-nitrosobenzene	3.07	171.5
1,3-dichloro-2-propanol	0.71	-4
1,3-dichloro-4-fluorobenzene	3.45	-23
1,3-dichloro-5,5-dimethylhydantoin	-1.48	132
1,3-dichloro-5-iodobenzene	4.07	57
1,3-dichloro-5-nitrobenzene	3.08	63.5
1,3-dichloroacetone	0.72	44
1,3-dichlorobenzene	3.45	-25
1,3-dichloropropene, cis trans	2.07	-84
1,3-diethoxybenzene	2.78	11
1,3-difluorobenzene	2.25	-59
1,3-dihydroxyacetone dimer	-1.91	78.5
1,3-dihydroxynaphthalene	2.02	124.5
1,3-diiodobenzene	3.8	36
1,3-diiodopropane	3.21	-20
1,3-diisopropylbenzene	4.71	-63
1,3-dimethoxybenzene	2	-52
1,3-dimethyl-2,4-dioxo-7-n-propyl-2,3,4,7-tetrahydropyrrolo(2,3-d)pyrimidine-6-carboxylic acid	0.7	139
1,3-dimethyl-2-imidazolidinone	-0.53	8
1,3-dimethyl-3,4,5,6-tetrahydro-2(1h)-pyrimidinone	-0.29	-23
1,3-dimethyl-6-methylamino-2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-	-1.11	203

carboxaldehyde		
1,3-dimethylbarbituric acid	-0.67	122
1,3-dimethyluracil	-0.98	120.5
1,3-di-n-butyl-2-thiobarbituric acid	2.7	62
1,3-dinitrobenzene	1.7	89
1,3-di-o-tolylguanidine	2.9	177
1,3-dioxolane	-0.61	-95
1,3-diphenoxy-2-propanol	2.7	82
1,3-diphenoxybenzene	4.96	60
1,3-diphenyl-1,3-propanedione	3.14	78
1,3-diphenyl-1-butanone	4.04	70
1,3-diphenylacetone	3.24	34
1,3-diphenylguanidine	2.67	149
1,3-diphenylisobenzofuran	6.15	134.5
1,3-di-tert-butylbenzene	5.58	9.5
1,3-dithiane	1.58	53.5
1,3-indanedione	1.54	130
1,3-phenylene diisocyanate	1.21	48
1,3-phenylenediacetic acid	1.3	175
1,3-phenylenediacetonitrile	0.72	33.5
1,3-propanediol	-1.18	-26
1,3-propanediol di-p-toluenesulfonate	1.68	91
1,3-propanedithiol	1.13	-79
1,3-propanesultone	-0.86	31.5
1,4,10,13-tetrathia-7,16-diazacyclooctadecane	1.75	130
1,4,5,6-tetrahydro-6-oxopyridazine-3-carboxylic acid	-1.49	197
1,4,6,7-tetramethylnaphthalene	5.28	63.5
1,4,8,11-tetraazacyclotetradecane	-0.66	186
1,4,8,11-tetraazatricyclo(9.3.1.1(4,8))hexadecane	0.34	84
1,4,8,11-tetrakis(ethoxycarbonylmethyl)-1,4,8,11-tetraazacyclotetradecane	1.49	88
1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane	1.25	35
1,4,8-tri-boc-1,4,8,11-tetraazacyclotetradecane	2.57	51
1,4-benzenedimethanol	0.17	119
1,4-benzenedithiol	1.81	97
1,4-benzodioxan-6-amine	1.17	28
1,4-benzodioxane-2-carboxylic acid	0.99	124
1,4-benzodioxane-2-thiocarboxamide	1.36	174
1,4-benzodioxane-6-carboxaldehyde	1.12	50
1,4-benzodioxane-6-sulfonyl chloride	1.76	66
1,4-bipiperidine	1.48	68
1,4-bis(1-hydroxycyclohexyl)-1,3-butadiyne	3.08	174.5
1,4-bis(2,2,2-trifluoroethoxy)benzene	3.49	76
1,4-bis(2-hydroxyisopropyl)benzene	2.13	144
1,4-bis(2-methylstyryl)benzene	6.9	181.5
1,4-bis(2-phenylethyl)benzene	6.82	89
1,4-bis(3-aminopropyl)piperazine	-0.67	14

1,4-bis(4-methyl-5-phenyloxazol-2-yl)benzene	6.45	234
1,4-bis(5-phenyloxazol-2-yl)benzene	5.76	242
1,4-bis(diphenylphosphino)butane	7.61	134
1,4-bis(glycidyloxy)benzene	1.28	111
1,4-bis(phenylethynyl)benzene	5.98	177
1,4-bis(trifluoromethyl)benzene	3.66	-1
1,4-bis(trimethylsilyl)-1,3-butadiyne	3.67	111.5
1,4-bis((trimethylsilyl)ethynyl)benzene	4.73	120
1,4-butanediol	-0.63	19.5
1,4-cyclohexadiene	2.31	-49
1,4-cyclohexanedione	0.1	77.5
1,4-diacetoxy-2-butyne	1.31	27.5
1,4-diacetoxybenzene	1.59	120.5
1,4-diacetoxybutane	1.06	12.5
1,4-diacryloylpiperazine	-0.27	93
1,4-diaminoanthraquinone	3	262.5
1,4-diaminobutane	-0.98	26.5
1,4-diazabicyclo(2.2.2)octane	-0.53	157.5
1,4-dibenzoylbenzene	4.64	163
1,4-dibenzyloxybenzene	4.99	126.5
1,4-dibromo-2,3-butanedione	0.78	117.5
1,4-dibromo-2,5-difluorobenzene	3.57	62
1,4-dibromo-2,5-dimethoxybenzene	3.72	146
1,4-dibromo-2-fluorobenzene	3.65	34
1,4-dibromo-2-nitrobenzene	3.31	83.5
1,4-dibromobenzene	3.71	88
1,4-dibromobutane	2.98	-20
1,4-dibromonaphthalene	4.84	81
1,4-dibromopentane	3.54	-34
1,4-dichloro-2-fluorobenzene	3.44	4
1,4-dichloro-2-iodobenzene	4.07	20.5
1,4-dichloro-2-nitrobenzene	3.04	55
1,4-dichloro-5,6,7,8-tetrahydro-5,8-ethanophthalazine	3.92	209.5
1,4-dichlorobenzene	3.46	54
1,4-dichlorobutane	2.51	-38
1,4-dicyclohexylbenzene	7.45	104
1,4-diethoxybenzene	2.8	70
1,4-diethylbenzene	4.36	-43
1,4-difluoro-2,5-dimethoxybenzene	2.16	120.5
1,4-difluoro-2-nitrobenzene	1.9	-12
1,4-difluorobenzene	2.26	-13
1,4-diformylpiperazine	-1.48	127.5
1,4-dihydroxyanthraquinone	2.98	196.5
1,4-diiodobenzene	3.8	130
1,4-diiodobutane	3.56	6
1,4-diisopropylbenzene	4.7	-17

1,4-dimethoxy-2-fluorobenzene	2.21	24.5
1,4-dimethoxybenzene	2.05	56
1,4-dimethoxynaphthalene	3.2	84.5
1,4-dimethylpiperazine	-0.01	-1
1,4-dinitrobenzene	1.7	174
1,4-di-o-tosyl-2,3-o-isopropylidene-l-threitol	1.99	90
1,4-dioxane	-0.23	11.8
1,4-dioxane-2,3-diol	-1.47	101
1,4-dioxane-2,5-dione	-0.67	82
1,4-diphenoxybenzene	4.97	72.5
1,4-diphenyl-1-butanone	3.85	55
1,4-diphenylbutadiyne	4.55	86.5
1,4-dipropionyloxybenzene	2.46	113
1,4-di-tert-butylbenzene	5.68	77
1,4-dithio-dl-threitol	0.18	41.5
1,4-dithioerythritol	0.18	83
1,4-naphthoquinone	1.61	122
1,4-oxathiane 4,4-dioxide	-1.36	132
1,4-oxazepan-5-one	-1.06	81
1,4-phenylene diisothiocyanate	3.96	130.5
1,4-phenylenediacetic acid	1.34	254
1,4-phenylenediacetonitrile	0.75	96
1,4-piperazinedipropionitrile	0.24	64.5
1,5,5-trimethylhydantoin	0.03	162.5
1,5-bis(diphenylphosphino)pentane	8.17	47
1,5-diaminonaphthalene	1.49	190.5
1,5-diaminopentane	-0.27	9
1,5-dibromopentane	3.51	-34
1,5-dichloro-2,4-dinitrobenzene	2.8	100.5
1,5-dichloroanthraquinone	4.14	247
1,5-dichloropentane	3.11	-72
1,5-difluoro-2,4-dinitrobenzene	1.56	74
1,5-dimethylnaphthalene	4.37	80
1,5-dinitronaphthalene	2.68	216
1,5-hexadiene	3.05	-141
1,5-pentamethylene-1h-tetrazole	0.56	60
1,5-pentanediol	-0.1	-16
1,5-pentanedithiol	2.01	-72
1,6-anhydro-beta-D-glucopyranose	-2.18	182
1,6-diaminohexane	0.27	41
1,6-dibromo-2-hydroxynaphthalene-3-carboxylic acid	4.42	251
1,6-dibromohexane	4.16	-2
1,6-dichlorohexane	3.6	-13
1,6-dicyanohexane	0.75	-3
1,6-dihydroxynaphthalene	1.99	138
1,6-diisocyanatohexane	1.88	-67

1,6-dimethoxynaphthalene	3.21	58.5
1,6-diphenoxy-2,4-hexadiyne	4.46	81.5
1,6-hexanediol	0.59	41.5
1,6-hexanedithiol	2.53	-21
1,7-diaminoheptane	0.79	28
1,7-dihydroxynaphthalene	2	182
1,7-heptanediol	1.16	17.5
1,7-phenanthroline	2.04	79
1,8,9-trihydroxyanthracene	2.73	179
1,8-bis(dimethylamino)naphthalene	3.85	49
1,8-cineole	3.36	1
1,8-diaminonaphthalene	1.22	63
1,8-diaminooctane	1.29	52
1,8-diazabicyclo(5.4.0)undec-7-ene	1.6	-70
1,8-dibenzyl-1,4,8,11-tetraazacyclotetradecane	2.28	67.5
1,8-dibromooctane	5.18	15.5
1,8-dichloroanthraquinone	4.14	202
1,8-dichlorooctane	4.63	-8
1,8-naphthalic anhydride	2.42	271
1,8-naphthalimide	2.06	301
1,8-nonadiyne	3.09	-21
1,8-octanediol	1.63	59.5
1,9-diaminononane	1.76	38
1,9-diphenyl-1,3,6,8-nonatetraen-5-one	5.52	142
1,9-nonanediol	2.11	46.5
1-(3,5-bis(trifluoromethyl)phenyl)ethanol	3.1	72
1-(3,5-bis(trifluoromethyl)phenyl)pyrrole	4.1	42
10,11-dihydrocarbamazepine	2.36	205
10,12-docosadiynedioic acid	5.37	111
10,12-pentacosadiynoic acid	8.19	63.5
10,12-tricosadiynoic acid	7.64	57
10-hydroxybenzo(h)quinoline	3.16	104
10-methylphenothiazine	4.13	101.5
10-phenyl-1-decanol	5.82	36
10-undecen-1-ol	4.58	-3
10-undecenoic acid	3.84	23.5
10-undecynoic acid	3.13	41.5
11-heneicosanol	9.06	72
12-aminododecanoic acid	0.25	186
12-hydroxystearic acid	6.61	74.5
12-tricosanone	9.5	67
14-heptacosanone	10.22	77.5
15-hydroxypentadecanoic acid	5.2	86
16-hydroxyhexadecanoic acid	5.77	99
18-crown-6	-0.39	39
18-pentatriacontanone	10.95	86.5

1-acetamidoadamantane	2.61	147.5
1-acetyl-2-naphthol	2.91	65
1-acetyl-3-thiosemicarbazide	-1.22	166.5
1-acetyl-4-(4-hydroxyphenyl)piperazine	1.17	182.5
1-acetyl-5-bromo-7-nitroindoline	2.34	197
1-acetyl-5-bromoindoline	2.13	119.5
1-acetyl-5-nitroindoline	1.31	176.5
1-acetylimidazole	-0.33	101
1-acetylisatin	0.72	142
1-acetylnaphthalene	2.97	10
1-acetylpiperazine	-1.03	32
1-acetylpiperidine-4-carbonyl chloride	0.72	132
1-acetylpiperidine-4-carboxylic acid	-0.3	182
1-acetylpyrene	4.99	87.5
1-adamantaneacetic acid	2.77	137
1-adamantaneethanol	3.34	74
1-adamantanemethanol	2.7	116.5
1-amino-2,4-dibromoanthraquinone	3.74	227
1-amino-4-hydroxyanthraquinone	2.97	208
1-amino-5-chloroanthraquinone	4	207
1-aminoanthraquinone	3.21	253.5
1-aminoindane	1.5	2
1-aminopyrene	4.26	117.5
1-aza-18-crown-6	-0.76	47.5
1-benzhydrylpiperazine	2.53	91.5
1-benzoyl-4-piperidone	1.03	54.5
1-benzoylnaphthalene	4.4	75.5
1-benzoylpiperidine	2.18	49
1-benzyl-1,2,3-triazole-4,5-dicarboxylic acid	0.16	180
1-benzyl-1,4,7,10-tetraazacyclododecane	0.09	85
1-benzyl-3-hydroxy-1h-indazole	3.35	165
1-benzyl-4-boc-piperazine	2.92	72
1-benzyl-4-cyano-4-hydroxypiperidine	1.18	97
1-benzyl-4-hydroxypiperidine	1.45	62
1-benzyl-5-phenylbarbituric acid	1.97	164
1-benzylimidazole	1.58	70.5
1-benzyloxy-3-iodobenzene	4.48	50.5
1-benzyloxy-4-bromobenzene	4.53	62
1-benzyloxy-4-iodobenzene	4.49	62
1-benzyloxycarbonyl-4-piperidone	1.12	39.5
1-boc-2-(hydroxydimethylsilyl)pyrrole	2.7	55
1-boc-2-piperidone	1.79	35.5
1-boc-3-azetidinone	0.75	50.5
1-boc-3-cyanoazetidine	1.24	69.5
1-boc-3-hydroxyazetidine	0.69	40
1-boc-3-hydroxypiperidine	1.51	68

1-boc-3-oxopiperazine	0.48	158
1-boc-3-piperidone	1.19	38
1-boc-3-pyrrolidinone	0.83	36
1-boc-4-cyanopiperidine	1.94	46.5
1-boc-4-hydroxypiperidine	1.45	63
1-boc-4-piperidinemethanol	1.83	80
1-boc-4-piperidone	1.08	74
1-boc-6-amino-1h-indazole	2.33	171.5
1-boc-azetidine-3-carboxylic acid	1.11	101.5
1-boc-imidazole	1.58	46
1-boc-indoline	3.01	47
1-boc-isonipecotic acid	1.66	150
1-boc-nipecotic acid ethyl ester	2.13	33
1-boc-piperazine	0.58	46
1-boc-pyrrole-2-carboxaldehyde	2.23	50.5
1-bromo-2,3,5,6-tetramethylbenzene	4.55	60
1-bromo-2,3,5-trichlorobenzene	4.68	59
1-bromo-2,3-dichlorobenzene	4.21	58
1-bromo-2,4,5-trifluorobenzene	2.99	-19
1-bromo-2,4-dichlorobenzene	4.2	26.5
1-bromo-2,4-difluorobenzene	2.98	-4
1-bromo-2,4-dimethoxybenzene	2.94	25
1-bromo-2,4-dinitrobenzene	2.32	71.5
1-bromo-2,5-difluoro-4-nitrobenzene	2.51	56
1-bromo-2-chloro-4-nitrobenzene	3.26	60.5
1-bromo-2-chlorobenzene	3.61	-13
1-bromo-2-chloroethane	1.65	-18
1-bromo-2-ethylbenzene	4.04	-68
1-bromo-2-fluoro-4-iodobenzene	3.46	36
1-bromo-2-fluorobenzene	2.91	-8
1-bromo-2-hexadecanone	7.41	56
1-bromo-2-iodobenzene	3.7	9.5
1-bromo-2-methoxynaphthalene	4.21	79.5
1-bromo-2-methylpropane	2.57	-118
1-bromo-2-naphthol	3.64	78.5
1-bromo-2-nitrobenzene	2.59	42
1-bromo-3,3-diphenylpropane	5.32	40.5
1-bromo-3,5-bis(trifluoromethyl)benzene	4.18	-16
1-bromo-3,5-dichlorobenzene	4.22	75
1-bromo-3,5-difluorobenzene	3	-27
1-bromo-3,5-di-tert-butylbenzene	6.95	64
1-bromo-3-chlorobenzene	3.59	-22
1-bromo-3-chloropropane	2.12	-59
1-bromo-3-fluorobenzene	3.02	-8
1-bromo-3-iodobenzene	3.69	-9
1-bromo-3-methylbutane	3	-112

1-bromo-3-phenoxypropane	3.12	9.5
1-bromo-4-chloro-2-nitrobenzene	3.2	70
1-bromo-4-chlorobenzene	3.63	65
1-bromo-4-fluoro-2-nitrobenzene	2.59	38
1-bromo-4-fluorobenzene	2.98	-16
1-bromo-4-fluoronaphthalene	4.24	35
1-bromo-4-iodobenzene	3.69	91
1-bromo-4-isopropylbenzene	4.24	-12
1-bromo-4-nitrobenzene	2.66	125.5
1-bromo-4-tert-butylbenzene	4.94	15.5
1-bromoadamantane	4.7	119
1-bromobutane	2.73	-112
1-bromodecane	5.92	-30
1-bromododecane	6.8	-10
1-bromoheptane	4.4	-58
1-bromohexadecane	7.61	17
1-bromohexane	3.88	-85
1-bromonaphthalene	3.99	-1
1-bromooctadecane	8.22	27.5
1-bromooctane	4.91	-55
1-bromopentadecane	7.36	18.5
1-bromopentane	3.27	-95
1-bromoperfluorooctane	4.74	6
1-bromopropane	2.18	-110
1-bromopyrene	6.04	94.5
1-bromotetradecane	7.31	5
1-bromoundecane	6.45	-9
1-butanefonyl chloride	1.43	-29
1-butanethiol	2.51	-116
1-butanol	0.84	-89.5
1-chloro-2,4-bis(trifluoromethyl)benzene	4.31	-59
1-chloro-2,4-difluoro-3-nitrobenzene	2.44	47
1-chloro-2,4-difluorobenzene	2.93	-26
1-chloro-2,4-dinitrobenzene	2.29	50
1-chloro-2-fluorobenzene	2.81	-43
1-chloro-2-iodobenzene	3.63	1
1-chloro-2-methylpropane	2.29	-131
1-chloro-2-nitrobenzene	2.48	32.5
1-chloro-3,4-dinitrobenzene	2.24	22.5
1-chloro-3,5-dibromobenzene	4.36	92.5
1-chloro-3,5-dimethoxybenzene	2.75	34
1-chloro-3-methylbutane	2.81	-104
1-chloro-3-nitrobenzene	2.49	45
1-chloro-4-fluoro-2-nitrobenzene	2.52	38
1-chloro-4-fluorobenzene	2.85	-22
1-chloro-4-iodobenzene	3.66	54.5

1-chloro-4-nitrobenzene	2.56	84
1-chloroacetyl-3-pyrazolidinone	-1.1	145.5
1-chloroadamantane	4.35	165
1-chloroanthraquinone	3.53	160
1-chlorobutane	2.37	-123
1-chloroethyl chloroformate	1.4	-65
1-chlorohexadecane	8.81	9
1-chlorohexane	3.63	-94
1-chloroisoquinoline	2.73	34
1-chloronaphthalene	3.95	-8
1-chlorooctane	4.82	-58
1-chloropentane	3.12	-99
1-chlorophthalazin-4-one	0.53	272
1-chlorophthalazine	1.65	110.5
1-cyano-1-cyclopropanecarboxylic acid	0.04	146
1-cyanoacetyl-3,5-dimethyl-1h-pyrazole	1.01	120
1-cyanomethylpiperidine	1	25
1-cyclohexene-1-acetic acid	1.85	33
1-cyclohexene-1-carboxylic acid	1.65	32
1-cyclohexyl-2-pyrrolidinone	1.86	12.5
1-cyclopentene-1-carboxylic acid	1.09	119
1-cyclopentyl-2,2-dimethyl-1-propanol	3.15	49
1-decanesulfonyl chloride	4.45	32
1-decanethiol	6.24	-26
1-decanol	4.24	6
1-decene	5.63	-66
1-decyne	5	-44
1-difluoromethoxy-4-nitrobenzene	2.13	34
1-dimethylamino-2-nitroethylene	-0.48	103
1-dimethylamino-2-propanol	-0.06	-85
1-dodecanesulfonyl chloride	5.4	40.5
1-dodecanethiol	7.13	-7
1-dodecanol	5.36	25.5
1-dodecene	6.53	-37
1-dodecyne	6.03	-19
1-eicosanol	8.9	64
1-ethoxy-2-propanol	0.14	-100
1-ethyl-2-phenylindole	5.28	85.5
1-ethyl-3-methyl-1h-pyrazole-5-carboxylic acid	0.66	138.5
1-ethyl-4-((4-methoxyphenyl)ethynyl)benzene	4.99	35
1-ethyl-4-((4-n-hexylphenyl)ethynyl)benzene	7.14	10
1-ethyl-4-((4-n-propylphenyl)ethynyl)benzene	5.89	50
1-ethyl-4-((p-tolyl)ethynyl)benzene	5.14	72.5
1-ethyl-4-iodobenzene	3.93	-17
1-ethylpiperazine-2,3-dione	-0.87	110
1-ethylpiperidine	2.11	-20

1-ethynylcyclohexanol	1.09	31.5
1-ethynylcyclopentanol	1.05	25
1-ethynylpyrene	5.13	114
1-fluoro-2,4-dinitrobenzene	1.66	27
1-fluoro-2-iodobenzene	2.8	-41.5
1-fluoro-2-nitrobenzene	1.84	-8
1-fluoro-3,5-dimethyl-2-nitrobenzene	2.51	55.5
1-fluoro-3-iodo-5-nitrobenzene	2.71	77.75
1-fluoro-3-iodobenzene	2.88	-42
1-fluoro-3-nitrobenzene	1.88	2
1-fluoro-4-iodobenzene	2.93	-20
1-fluoro-4-nitrobenzene	1.97	23
1-fluoronaphthalene	3.37	-10
1-formylpiperidine	0.21	-31
1h-1,2,3-triazole	-0.73	24
1h-1,2,4-triazole-1-acetic acid	-1.25	203
1h-benzotriazole	1.19	97.5
1-heptadecanol	7.82	53.5
1-heptanethiol	4.28	-43
1-heptanol	2.53	-34
1-heptene	4	-119
1-heptylamine	2.57	-23
1-heptyne	3.26	-81
1-hexadecanesulfonyl chloride	7.18	57
1-hexadecanethiol	8.44	21
1-hexadecanol	7.17	49
1-hexadecene	8.11	4
1-hexadecyne	7.47	14.5
1-hexanethiol	3.65	-81
1-hexanol	2.03	-52
1-hexene	3.38	-140
1-hexylamine	1.98	-19
1-hexyne	2.63	-132
1h-indazole	1.61	147.5
1h-indene	3.04	-2
1h-pyrazole	0.03	68
1h-pyrazole-4-carboxylic acid	-0.25	282
1-hydroxycyclohexyl phenyl ketone	2.04	47.5
1-hydroxyisoquinoline	2.02	213.5
1-hydroxymethyl-5,5-dimethylhydantoin	-0.53	105
1-indanol	1.59	52
1-indanone	1.77	40
1-iodo-2,3,4,5-tetramethylbenzene	4.29	31
1-iodo-2,4-dinitrobenzene	2.43	88.5
1-iodo-2-methylpropane	3.3	-93
1-iodo-2-nitrobenzene	2.83	50

1-iodo-3,5-dinitrobenzene	2.46	101
1-iodo-3-nitrobenzene	2.82	36.5
1-iodo-4-nitrobenzene	2.92	174.5
1-iodobutane	3.11	-103
1-iododecane	6.03	-16
1-iodododecane	6.78	-3
1-iodoheptane	4.69	-48
1-iodohexadecane	8.25	22
1-iodohexane	4.19	-75
1-iodonaphthalene	4.06	4
1-iodooctane	5.17	-46
1-iodopentane	3.64	-86
1-iodopropane	2.65	-101
1-methoxy-2-propanol	-0.44	-100
1-methoxynaphthalene	3.34	5
1-methyl-1h-benzotriazole	0.99	64.5
1-methyl-1h-pyrazole-3-carboxylic acid	0.08	154
1-methyl-1h-pyrazole-5-carboxylic acid	-0.13	223.5
1-methyl-2-phenylindole	4.81	98.5
1-methyl-2-pyridone	-0.06	31
1-methyl-2-pyrrolidinone	-0.72	-24
1-methyl-2-quinolinone	1.27	75
1-methyl-3-n-propyl-2-pyrazolin-5-one	0.27	115
1-methyl-3-phenylpiperazine	0.94	58
1-methyl-3-trifluoromethyl-2-pyrazolin-5-one	0.7	179
1-methyl-4-(4-piperidinyl)piperazine	0.08	54.5
1-methyl-5-nitro-1h-indazole	1.68	160
1-methyl-6-nitro-1h-indazole	1.41	125.5
1-methylbenzimidazole	1.55	60.5
1-methylbenzimidazole-2-carboxaldehyde	1.4	119.5
1-methylcyclohexanecarboxylic acid	2.14	37.5
1-methylcyclohexanol	1.81	26
1-methylcyclopentanol	1.3	36.5
1-methylcyclopentene	2.89	-142
1-methylfluorene	4.56	85
1-methylhydantoin	-1.2	157.5
1-methylimidazole	-0.18	-6
1-methylimidazole-4,5-dicarbonitrile	-0.07	84.5
1-methylimidazole-4-carboxylic acid	-0.22	242
1-methylimidazole-5-carboxaldehyde	-0.68	54.5
1-methylindole-3-carboxaldehyde	1.66	69
1-methylisatin	0.68	131
1-methylisoquinoline	2.55	10
1-methylnaphthalene	3.84	-22
1-methylpiperazine	-0.92	-6
1-methylpiperidine	1.31	-50

1-methylpyrrole	1.31	-57
1-methylpyrrole-2-carboxylic acid	0.74	136.5
1-methylpyrrolidine	0.54	-90
1-methylsulfonyl-1h-benzotriazole	0.48	110
1-methylsulfonyl-4-nitrobenzene	0.62	137
1-methylthio-1-methylamino-2-nitroethylene	0	112.5
1-naphthaldehyde	2.96	1.5
1-naphthaleneacetylhydrazide	1.71	168
1-naphthaleneboronic acid	1.88	207
1-naphthalenemethanol	2.17	60.5
1-naphthoic acid	2.79	161
1-naphthoic hydrazide	1.48	167
1-naphthol	2.79	96
1-naphthoyl chloride	3.35	17.5
1-naphthyl acetate	2.9	44.5
1-naphthyl isocyanate	2.42	4
1-naphthyl isothiocyanate	4.33	55.5
1-naphthylacetamide	2.07	177
1-naphthylacetic acid	2.97	129.5
1-naphthylacetonitrile	2.83	34
1-n-butyl-4-((4-butylphenyl)ethynyl)benzene	7.04	41
1-n-butyl-4-((4-ethoxyphenyl)ethynyl)benzene	5.96	54
1-n-butyl-4-((4-methoxyphenyl)ethynyl)benzene	5.61	40
1-n-hexyl-4-((p-tolyl)ethynyl)benzene	6.6	42
1-n-hexyltheobromine	1.8	80.5
1-nitro-4-(trifluoromethoxy)benzene	2.76	15
1-nitro-4-n-propylbenzene	3.5	-14
1-nitronaphthalene	3.2	57
1-nitropropane	0.91	-108
1-nonanol	3.76	-7
1-nonylamine	3.69	-1
1-nonyne	4.45	-50
1-o-acetyl-2,3,5-tri-o-benzoyl-beta-D-ribofuranose	4.18	129
1-octadecanesulfonyl chloride	8.31	58
1-octadecanethiol	8.98	31.5
1-octadecanol	8.27	58
1-octadecene	9.03	16
1-octanesulfonyl chloride	3.43	14
1-octanethiol	4.95	-49
1-octanol	3.21	-16
1-octen-3-ol	2.43	-49
1-octene	4.61	-102
1-octylamine	3.24	-1
1-octyne	3.86	-60
1-pentadecanol	6.6	45.5
1-pentadecene	7.7	-4

1-pentadecyne	7.16	10
1-pentanethiol	3.02	-76
1-pentanol	1.47	-79
1-pentene	2.84	-138
1-pentenylboronic acid	1.48	80
1-pentylamine	1.39	-55
1-pentyne	2.13	-106
1-phenyl-1,2,3-butanetrione 2-oxime	1.21	129
1-phenyl-1,2-ethanediol	0.46	67
1-phenyl-2-propyn-1-ol	1.25	28
1-phenyl-2-pyrrolidinone	1.05	65.5
1-phenyl-3-pyrazolidinone	0.46	121.5
1-phenyl-3-trifluoromethyl-2-pyrazolin-5-one	2	193
1-phenylcyclohexanol	2.97	60
1-phenylcyclohexene	4.53	-11
1-phenylcyclopentanecarboxylic acid	3.04	159.5
1-phenylcyclopropanecarboxylic acid	2.08	87
1-phenylimidazole	1.65	13
1-phenylisatin	1.95	140.5
1-phenylpiperazine	1.54	18
1-phenylpyrrole	2.9	58.5
1-phenylsemicarbazide	0.12	172
1-piperonylpiperazine	0.42	42.5
1-propanethiol	1.72	-113
1-propanol	0.21	-127
1-propylamine	0.31	-83
1-pyrenebutyric acid	5.15	185
1-pyrenecarboxaldehyde	4.62	126.5
1-tert-butyl-2-imidazolidinone	0.5	137
1-tetradecanethiol	7.81	6.5
1-tetradecanol	6.21	38.5
1-tetradecene	7.27	-12
1-tetralone	2.29	7
1-thio-beta-D-glucose tetraacetate	1.67	116
1-tridecene	6.89	-23
1-trifluoromethylcyclopropane-1-carboxylic acid	1.09	88
1-trimethylsilyl-1-propyne	2.8	-69
1-tritylimidazole	4.72	222
1-undecanol	4.83	14
1-undecene	6.11	-49
1-undecyne	5.55	-25
2-(1,3-benzodioxol-5-yl)piperazine	-0.26	122
2-(1-boc-4-piperidinyloxy)-n,n-dimethylacetamide	1.31	58
2-(1-boc-4-piperidinyloxy)-n-cyclopropylacetamide	1.66	86
2-(1-boc-4-piperidinyloxy)-n-methylacetamide	1.05	95
2-(1-cyclohexenyl)ethylamine	1.76	-55

2-(1-naphthyl)ethanol	2.66	62
2-(1-piperazinyl)aniline	0.84	115
2-(1-piperazinyl)phenol	0.78	124.5
2-(1-piperazinyl)pyrimidine	0.32	33
2-(1-piperidinyl)aniline	2.76	45.5
2-(1-piperidinyl)benzotrile	3.06	43
2-(1-piperidinyl)phenol	3	74.5
2-(1-piperidinyl)thiazole-5-carboxaldehyde	2.02	48.5
2-(1-pyrrolidinyl)phenol	2.23	110.5
2-(1-pyrrolyl)benzoic acid	1.86	104
2-(2,2,2-trimethylacetamido)benzeneboronic acid	1.59	269.5
2-(2,4,5-trichlorophenoxy)propionic acid	3.88	178
2-(2,4-dichlorophenoxy)propionic acid	3.13	114
2-(2,4-dinitrobenzyl)pyridine	2.5	92
2-(2,6-dimethoxyphenyl)-4,4-dimethyl-2-oxazoline	2.62	69
2-(2-aminoethoxy)ethanol	-1.41	-11
2-(2-aminophenyl)benzimidazole	2.72	214
2-(2-carboxyvinyl)benzeneboronic acid	1.06	171
2-(2-chloro-4-methoxyphenyl)-3-oxobutyronitrile	2.1	79
2-(2-chlorophenoxy)ethylamine	1.46	39.5
2-(2-chlorophenyl)benzimidazole	4.14	234
2-(2-ethoxyphenoxy)ethyl bromide	3.26	42
2-(2-furyl)-1,3-diphenylimidazolidine	4.2	130
2-(2-furyl)piperazine	-0.21	86.5
2-(2-hydroxyethyl)pyridine	0.45	-8
2-(2-hydroxyphenyl)benzothiazole	4.04	132
2-(2-methoxyphenyl)-5-phenyl-1,3,4-oxadiazole	3.34	100
2-(2-methoxyphenyl)piperazine	0.35	79.5
2-(2-methyl-1,3-dioxolan-2-yl)benzeneboronic acid	0.82	110.5
2-(2-naphthoxy)ethanol	2.46	74
2-(2-naphthyl)piperazine	1.54	101.5
2-(2-n-butoxyethoxy)ethyl acetate	1.42	-32
2-(2-pyridyl)benzimidazole	2.55	223
2-(2-thienyl)piperazine	0.24	83
2-(2-thienyl)pyridine	2.79	62.5
2-(3,4-dimethoxyphenyl)ethanol	1.63	46
2-(3,4-dimethoxyphenyl)ethylamine	0.9	11
2-(3-chloro-4-fluorophenyl)indole	4.8	171.5
2-(3-chlorophenoxy)propionic acid	2.56	114.5
2-(3-pyridyl)benzimidazole	2.3	257
2-(3-thienyl)piperazine	0.24	97.5
2-(4-aminophenyl)-1,1,1,3,3,3-hexafluoro-2-propanol	2.72	150
2-(4-aminophenyl)ethanol	0.32	109
2-(4-aminophenyl)ethylamine	0.02	29.5
2-(4-benzyloxyphenyl)ethanol	3.29	86
2-(4-biphenyl)-2-propanol	3.89	91.5

2-(4-biphenyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole	6.16	137
2-(4-biphenyl)ethylamine	3.23	52
2-(4-bromophenyl)-5-(1-naphthyl)-1,3,4-oxadiazole	5.08	147.5
2-(4-bromophenyl)-5-phenyl-1,3,4-oxadiazole	3.93	169.5
2-(4-chloro-2-methylphenoxy)acetic acid hydrazide	1.36	150
2-(4-chloro-3-nitrobenzoyl)benzoic acid	3.19	199.5
2-(4-chlorobenzoyl)benzoic acid	3.3	150
2-(4-chlorobenzyl)pyridine	3.56	8
2-(4-chlorophenoxy)ethanol	1.91	30
2-(4-chlorophenoxy)isobutyric acid	2.81	119.5
2-(4-chlorophenoxy)nicotinic acid	2.69	158
2-(4-chlorophenyl)indole	4.7	206
2-(4-chlorophenylthio)-6-fluorobenzonitrile	4.8	69.5
2-(4-chlorophenylthio)benzaldehyde	4.75	72.5
2-(4-chlorophenylthio)nicotinic acid	3.3	220
2-(4-cyanophenyl)-5-n-pentyl-1,3-dioxane	3.89	57
2-(4-cyanophenyl)-5-n-propyl-1,3-dioxane	3.25	57.5
2-(4-ethoxyphenyl)ethanol	2.16	42
2-(4-ethylphenyl)-5-n-propylpyrimidine	3.98	42
2-(4-fluorophenoxy)nicotinic acid	2.32	183.5
2-(4-fluorophenyl)indole	4.14	188.5
2-(4-hydroxyphenyl)ethanol	0.85	90.5
2-(4-hydroxyphenyl)propionic acid	1.52	131
2-(4-methoxybenzoyl)thiophene	3.3	73
2-(4-methoxyphenyl)ethanol	1.61	28
2-(4-morpholinyl)-5-(trifluoromethyl)aniline	1.73	126.5
2-(4-morpholinyl)aniline	1.02	96.5
2-(4-n-hexyloxyphenyl)-5-n-octylpyrimidine	7.35	59.5
2-(4-pyridyl)benzimidazole	2.31	218.5
2-(4-tert-butylphenyl)ethanol	3.72	33
2-(4-toluoyl)benzoic acid	2.95	138
2(5h)-furanone	0.12	3.5
2-(5-isoxazolyl)-4-methylphenol	2.37	176
2-(5-isoxazolyl)phenol	2.07	184.5
2-(5-nitro-2-pyridyloxy)ethanol	0.67	113
2-(8-chloro-1-naphthylthio)acetic acid	3.76	156
2-(allylthio)nicotinic acid	1.44	146.5
2-(aminomethyl)pyridine	-0.19	-20
2-(boc-amino)-5-cyanopyridine	2.05	172.5
2-(boc-amino)benzeneboronic acid	1.51	124
2-(boc-amino)pyridine	2.29	93
2-(bromoacetyl)naphthalene	3.37	82.5
2-(bromoacetyl)thiophene	2.01	31
2-(bromomethyl)benzonitrile	2.75	72
2-(bromomethyl)benzothiazole	3.06	48
2-(bromomethyl)naphthalene	4.01	53

2-(carboxymethoxy)benzoic acid	1.03	189
2-(carboxymethylthio)benzoic acid	1.42	217.5
2-(diethylamino)ethanol	0.56	-70
2-(difluoromethoxy)benzoic acid	1.71	99
2-(dimethylamino)ethanol	-0.46	-60
2-(dimethylamino)ethyl acrylate	0.58	-60
2-(dimethylamino)ethyl methacrylate	0.87	-30
2-(diphenylphosphino)benzoic acid	4.94	177.5
2-(di-tert-butylphosphino)-2-(n,n-dimethylamino)biphenyl	7.4	115.5
2-(di-tert-butylphosphino)-2-methylbiphenyl	7.76	91.5
2-(ethoxycarbonyl)benzeneboronic acid	0.81	131.5
2-(ethoxycarbonyl)phenyl isocyanate	1.82	29
2-(ethylamino)ethanol	-0.49	-9
2-(ethylsulfonyl)ethanol	-0.64	38
2-(ethylthio)ethanol	0.61	-100
2-(ethylthio)nicotinic acid	1.51	185
2-(ethylthio)nicotinoyl chloride	2.29	51
2-(methacryloyloxy)ethyl 3,5-diaminobenzoate	1.09	91
2-(methacryloyloxy)ethyl 3,5-dinitrobenzoate	2.3	71
2-(methoxycarbonyl)benzeneboronic acid	0.34	69
2-(methoxycarbonyl)benzenesulfonamide	0.62	124
2-(methoxycarbonyl)phenyl isocyanate	1.38	47
2-(methylamino)ethanol	-1.05	-5
2-(methylamino)pyridine	1.13	14.5
2-(methylsulfonyl)acetanilide	0.59	145
2-(methylsulfonyl)benzoic acid	0.41	138.5
2-(methylsulfonyl)ethanol	-1.65	28.5
2-(methylsulfonyl)thiophene	0.74	47.5
2-(methylthio)benzeneboronic acid	1.25	160
2-(methylthio)benzimidazole	2.47	204
2-(methylthio)benzoic acid	2.24	167
2-(methylthio)benzotrile	1.95	35.5
2-(methylthio)naphthalene	4.02	62.5
2-(methylthio)nicotinic acid	0.83	216.5
2-(methylthio)nicotinoyl chloride	1.66	94
2-(methylthio)oxazolo(5,4-c)pyridine	1.33	80
2-(methylthio)pyrazine	0.99	44
2-(n-boc-methylamino)-5-iodo-3-methylpyridine	3.21	98.5
2-(n-hexyloxy)ethanol	1.82	-42
2-(nitromethylene)thiazolidine	-0.36	142
2-(n-propylthio)nicotinamide	1.57	147
2-(n-propylthio)nicotinic acid	1.96	161
2-(phenylsulfonyl)thiophene	1.82	123
2-(phthalimido)ethanesulfonyl chloride	1.01	158
2-(p-hydroxyphenylazo)benzoic acid	3.67	206
2-(p-toluenesulfonyl)ethanol	0.33	51.5

2-(p-tolyloxy)benzaldehyde	3.65	55
2-(trifluoromethoxy)benzamide	1.52	154
2-(trifluoromethoxy)benzeneboronic acid	1.89	119
2-(trifluoromethoxy)benzenesulfonamide	2.42	188.5
2-(trifluoromethoxy)benzenesulfonyl chloride	3.12	30.5
2-(trifluoromethoxy)benzoic acid	2.95	79
2-(trifluoromethoxy)phenylacetic acid	2.8	55
2-(trifluoromethyl)acetanilide	2.26	95.5
2-(trifluoromethyl)acetophenone	2.55	16
2-(trifluoromethyl)acrylic acid	1.59	50
2-(trifluoromethyl)aniline	2.24	-34
2-(trifluoromethyl)benzaldehyde	2.35	-40
2-(trifluoromethyl)benzamide	1.6	162.5
2-(trifluoromethyl)benzeneboronic acid	1.73	109
2-(trifluoromethyl)benzenesulfonamide	1.94	182
2-(trifluoromethyl)benzenesulfonyl chloride	2.92	23
2-(trifluoromethyl)benzoic acid	2.76	108.5
2-(trifluoromethyl)benzotrile	2.47	17.5
2-(trifluoromethyl)benzophenone	3.76	59.5
2-(trifluoromethyl)benzoyl chloride	2.82	-22
2-(trifluoromethyl)benzyl alcohol	2.08	4
2-(trifluoromethyl)benzyl bromide	3.62	28.5
2-(trifluoromethyl)cinnamic acid	3.23	202
2-(trifluoromethyl)nicotinic acid	1.63	186
4-aminobenzoic acid	0.78	187.5
5,5-diphenylhydantoin	2.26	295.5
acetanilide	1.05	114.5
adenosine	-1.21	235
antipyrine	1.01	112.5
benzamide	0.51	127
benzoic acid	1.72	122.5
chloramphenicol	1.15	150.5
flufenamic acid	4.6	134
griseofulvin	2.71	219
hydrochlorothiazide	-0.16	269
nalidixic acid	1.27	229
nicotinic acid	0.29	237.5
papaverine	4.19	146.5
perylene	6.34	278
pyrene	5.19	150
quinidine	2.82	170
salicylamide	0.74	140
salicylic acid	1.96	159
sulfacetamide	0.15	183
sulfadiazine	0.25	254.5
sulfamethazine	0.43	199.5

sulfanilamide	-0.16	165.5
thymine	-0.8	316.5
thymol	3.16	50.5
tolbutamide	2.04	129
triphenylene	5.77	196.5
uracil	-1.28	330

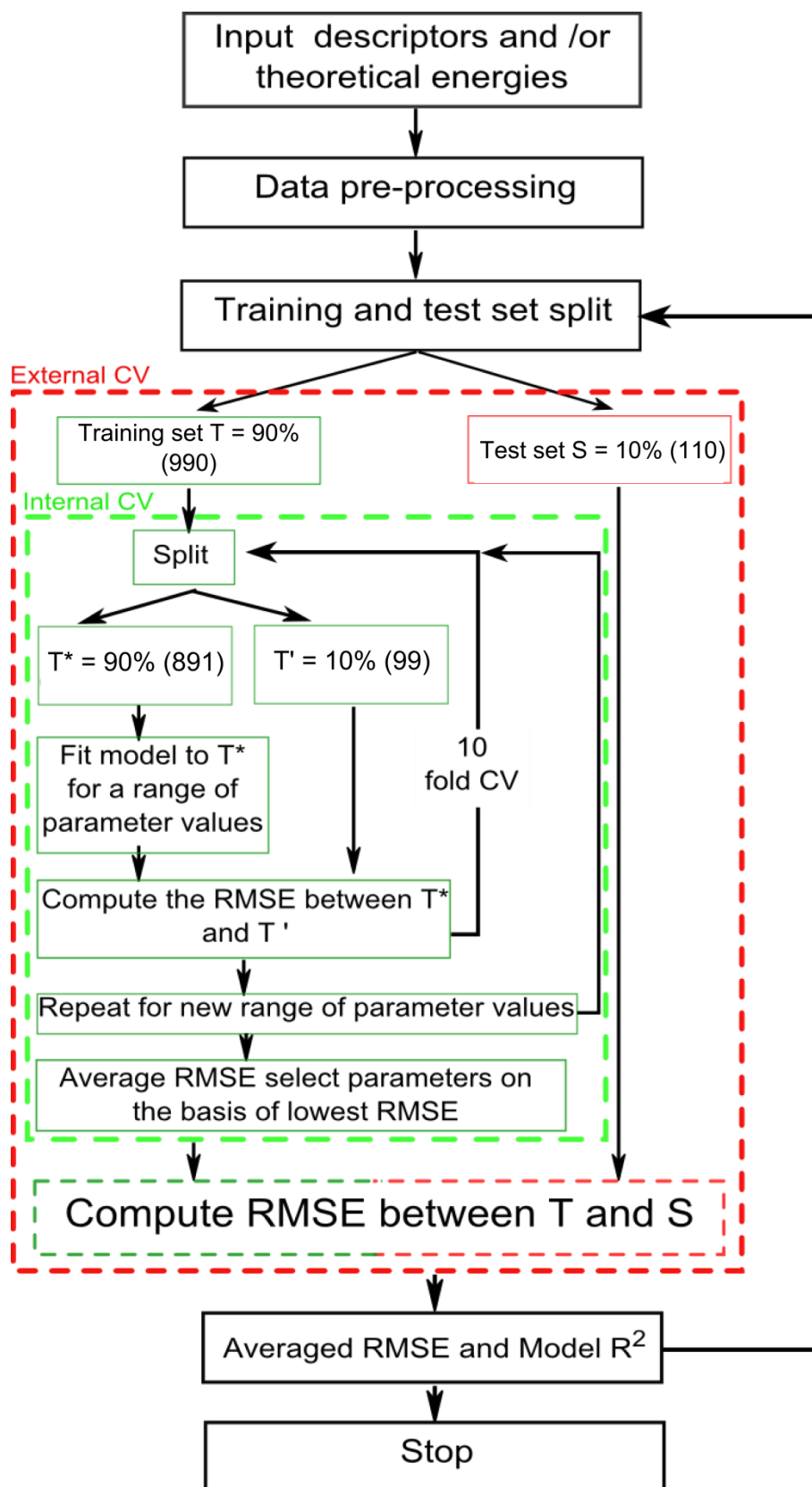


Figure S1. Machine learning workflow diagram. Inspired from the following references.[1, 2]

RF Melting Point Prediction Without the Xlog P Descriptor MP1100 Dataset

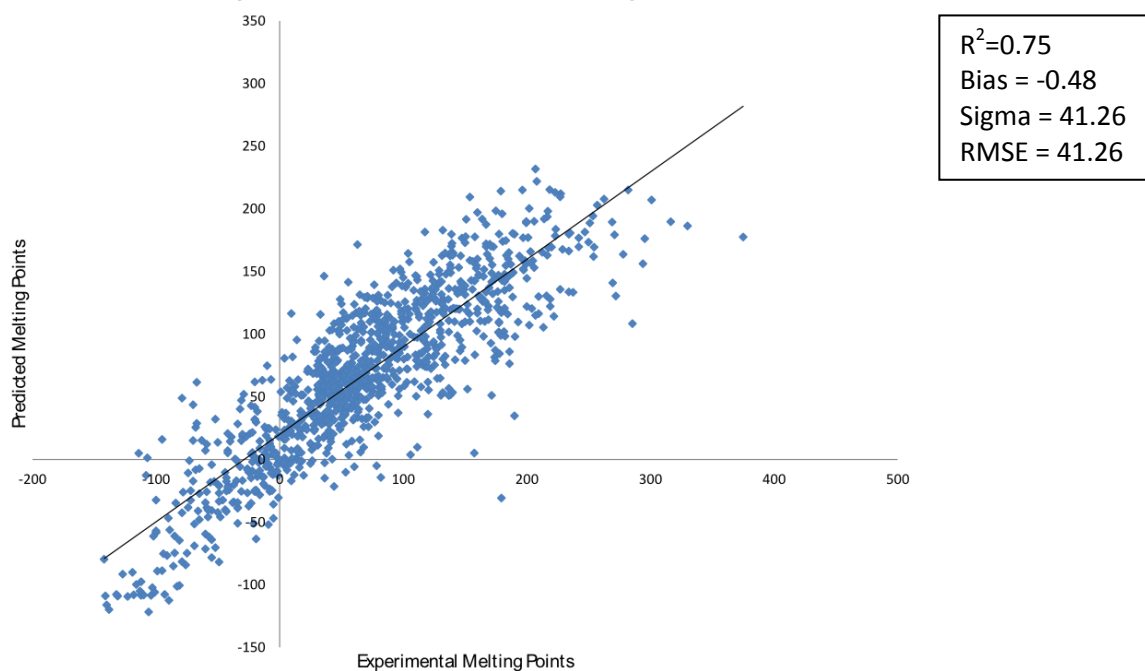


Figure S2. RF melting point prediction without the logP descriptor XlogP.

SVM Melting Point Predictions Without the Xlog P Descriptor MP1100 Dataset

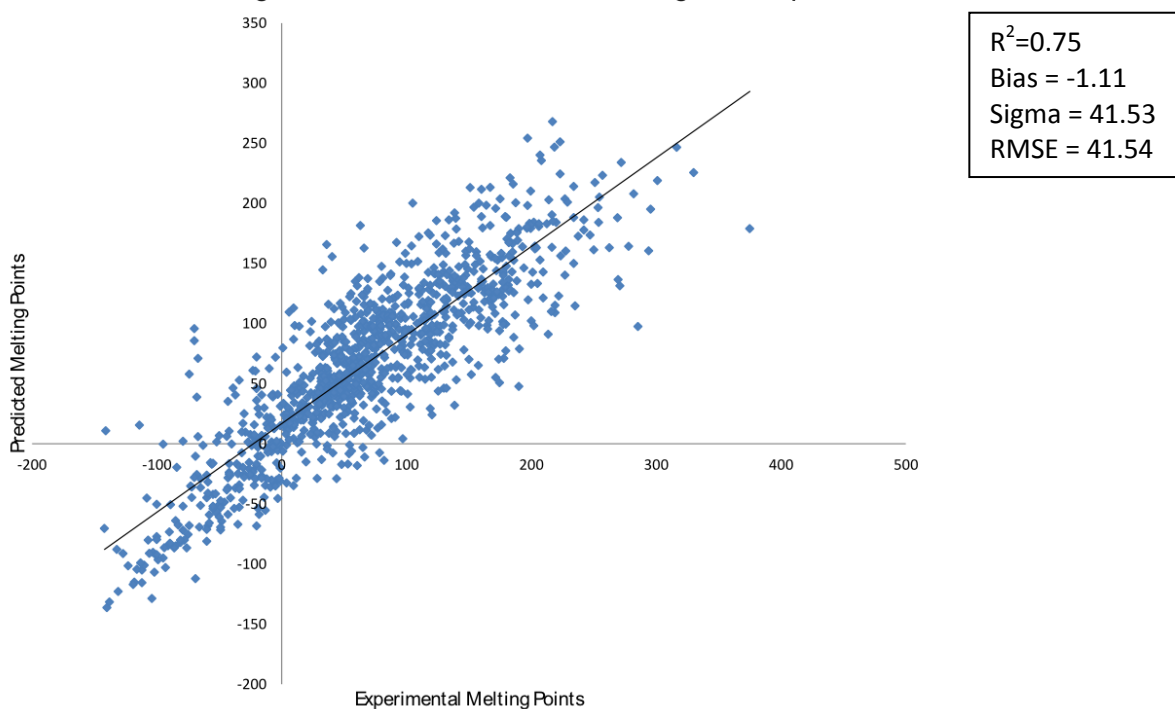


Figure S3. SVM melting point prediction without the logP descriptor XlogP.

PLSMelting Point Predictions Without the Xlog P Descriptor MP1100 Dataset

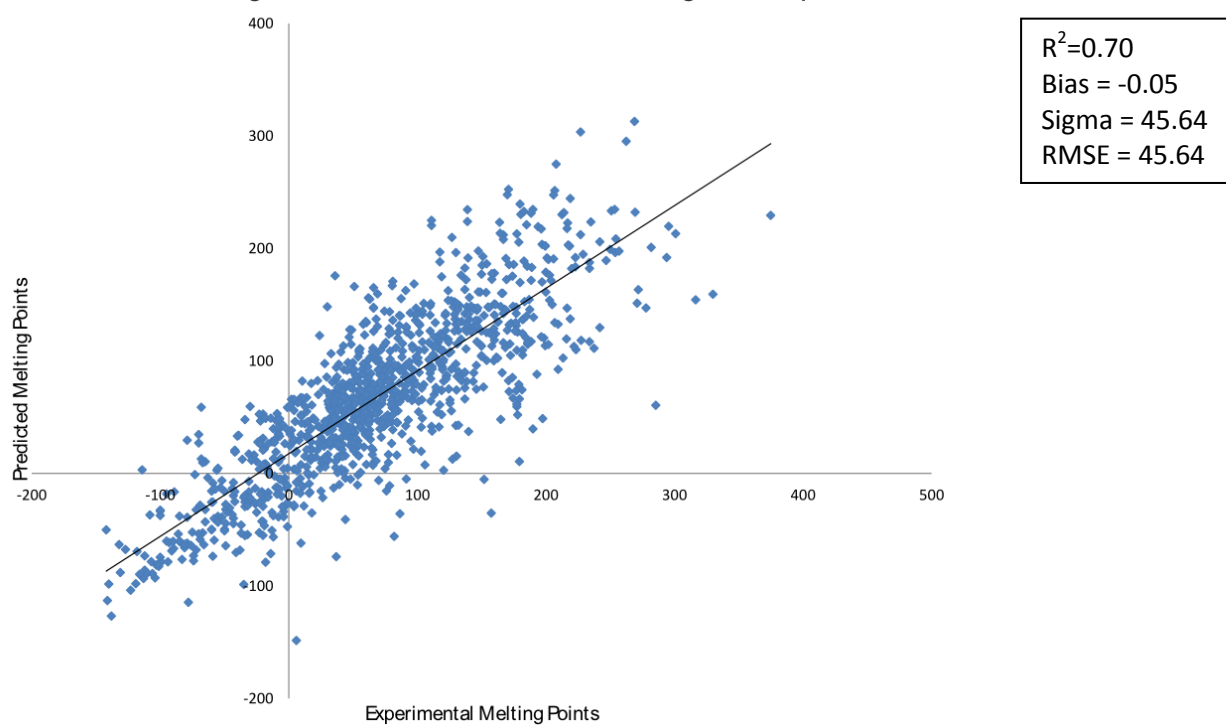


Figure S4. PLS melting point prediction without the logP descriptor XlogP.

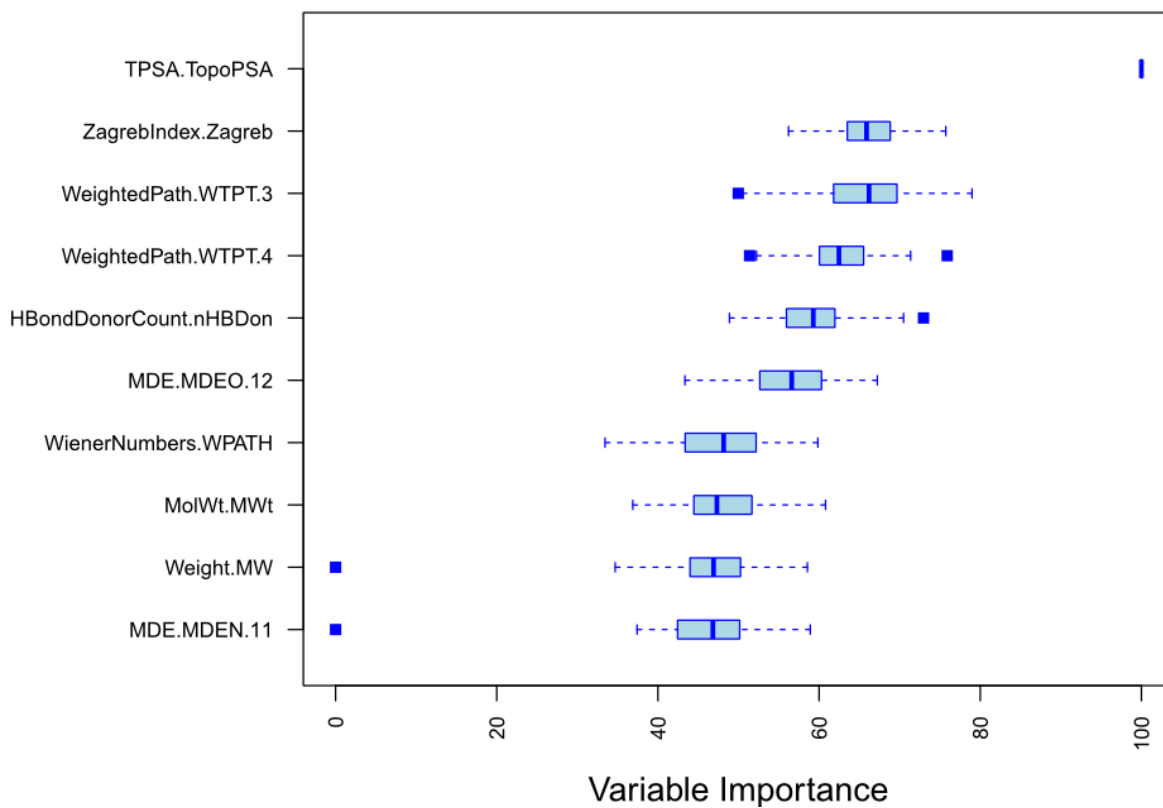


Figure S5. The most important descriptors in the RF model.

Table S2. The absolute differences between the LogS values predicted by the GSE using experimental MP (Exp logS) and machine learning MP's (pred logS).

Molecule	PLS logS AAE $ \log S(\text{Exp}^{\text{MP}}) - \log S(\text{Pred}^{\text{MP}}) $	RF logS AAE $ \log S(\text{Exp}^{\text{MP}}) - \log S(\text{Pred}^{\text{MP}}) $	SVM logS AAE $ \log S(\text{Exp}^{\text{MP}}) - \log S(\text{Pred}^{\text{MP}}) $
1,3,5-trichlorobenzene	0.36	0.27	0.22
1-Naphthol	0.21	0.57	0.34
4-Aminobenzoic acid	0.43	0.40	0.19
5,5-Diphenylhydantoin	0.72	1.22	1.05
Acetanilide	0.40	0.55	0.52
Adenosine	0.05	0.54	1.20
Antipyrine	0.11	0.34	0.18
Benzamide	0.34	0.38	0.45
Benzoic acid	0.37	0.11	0.20
Chloramphenicol	0.32	0.28	0.11
Flufenamic acid	0.45	0.31	0.50
Griseofulvin	0.80	0.92	1.04
Hydrochlorothiazide	0.49	0.78	0.83
Nalidixic acid	0.25	0.62	0.30
Nicotinic acid	1.27	1.02	0.70
Papaverine	0.33	0.08	0.22
Perylene	1.27	1.12	1.09
Pyrene	0.41	0.19	0.47
Quinidine	0.48	0.12	0.48
Salicylamide	0.09	0.21	0.37
Salicylic acid	0.32	0.07	0.07
Sulfacetamide	0.05	0.28	0.41
Sulfadiazine	0.46	0.86	0.49
Sulfamethazine	0.07	0.13	0.10
Sulfanilamide	0.05	0.13	0.38
Thymine	1.63	1.28	0.62
Thymol	0.28	0.07	0.27
Tolbutamide	0.11	0.16	0.33
Triphenylene	0.70	0.37	0.14
Uracil	1.71	1.45	1.01
Average	0.48	0.49	0.48

1. McDonagh, J.L., *Computing the Aqueous solubility of Organic Drug-Like Molecules and Understanding Hydrophobicity*, in *School of Chemistry*, 2015, University of St Andrews: Univeristy of St Andrews.
2. McDonagh, J.L., et al., *Uniting Cheminformatics and Chemical Theory To Predict the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules*. *Journal of Chemical Information and Modeling*, 2014. **54**(3): p. 844-856.