

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 |

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| (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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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-pentenediol | -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 |

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| 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 |

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| 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-acetylpirene | 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

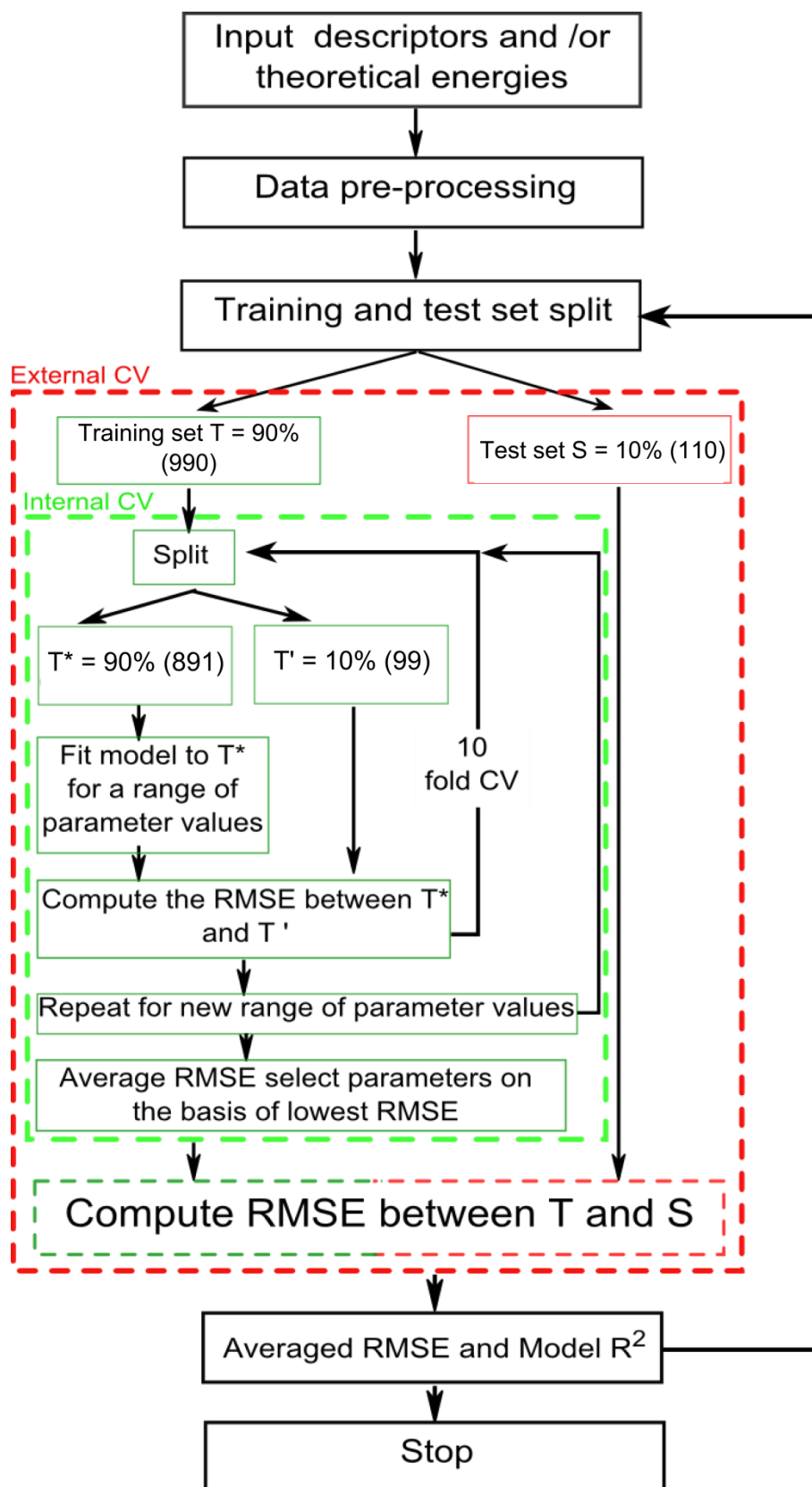


Figure S1. Machine learning workflow diagram. Inspired from the following references.[1, 2]

RF Melting Point Prediction Without the Xlog P Descriptor MP1100 Dataset

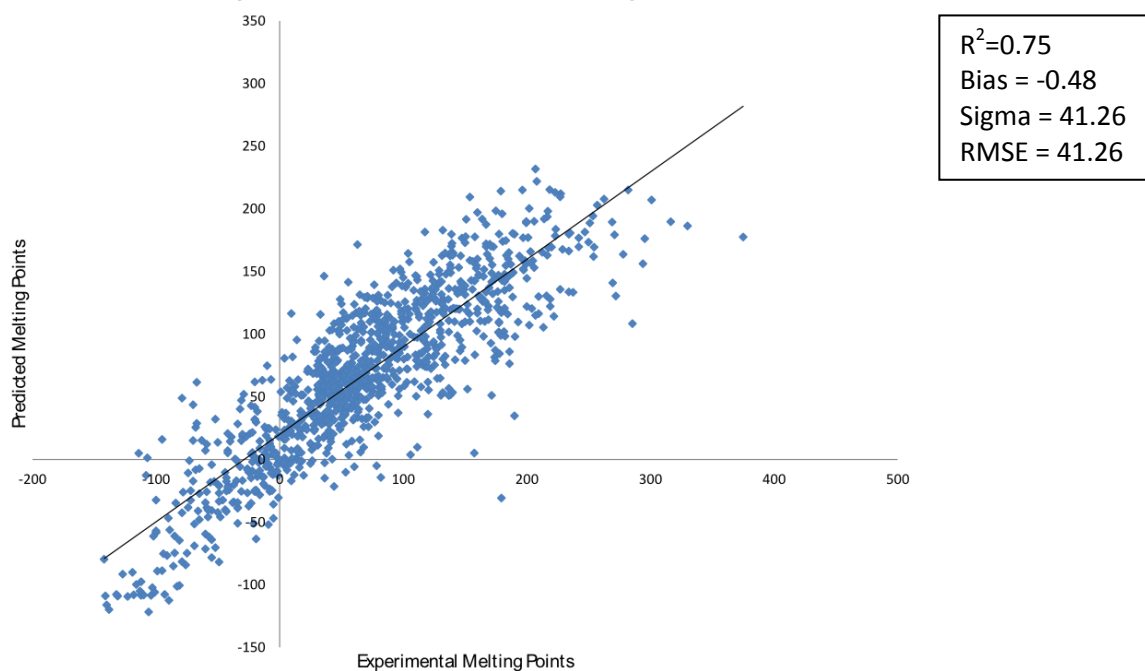


Figure S2. RF melting point prediction without the logP descriptor XlogP.

SVM Melting Point Predictions Without the Xlog P Descriptor MP1100 Dataset

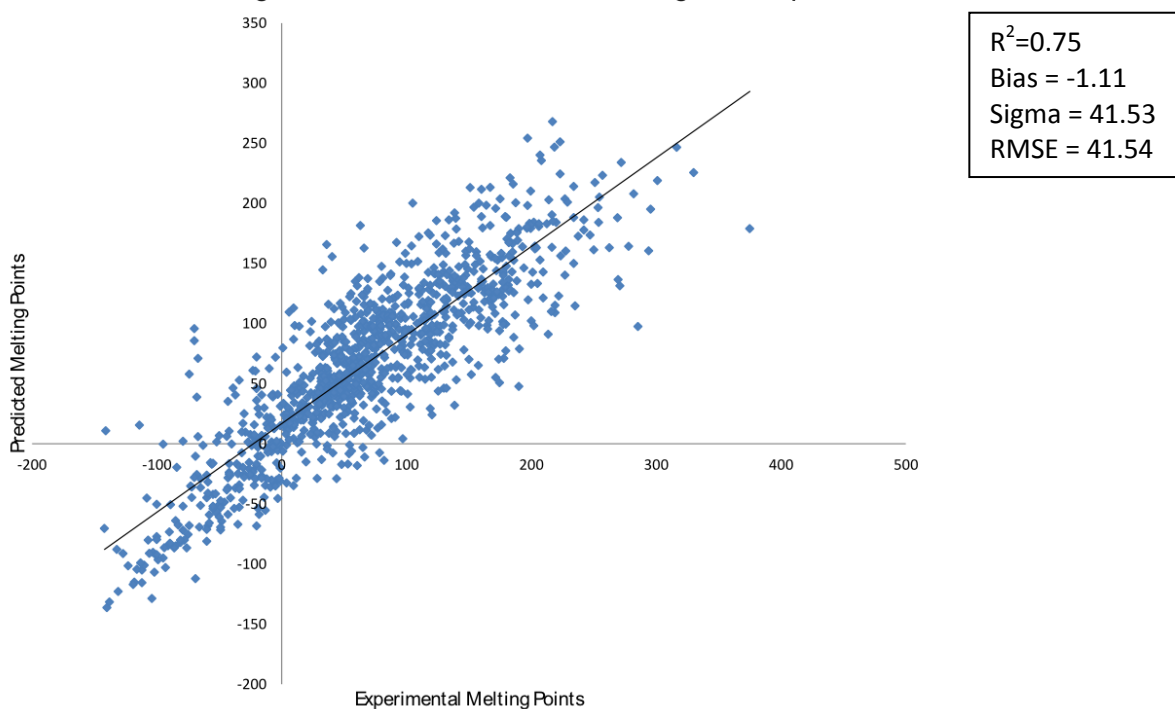


Figure S3. SVM melting point prediction without the logP descriptor XlogP.

PLSMelting Point Predictions Without the Xlog P Descriptor MP1100 Dataset

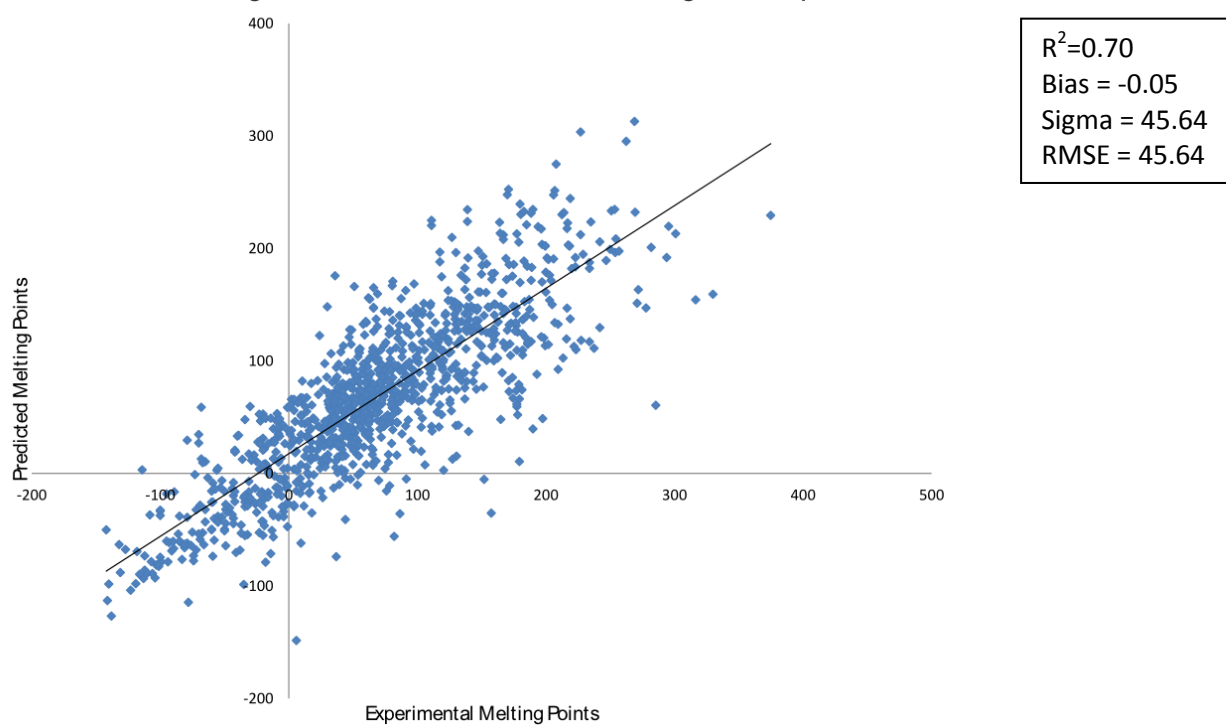


Figure S4. PLS melting point prediction without the logP descriptor XlogP.

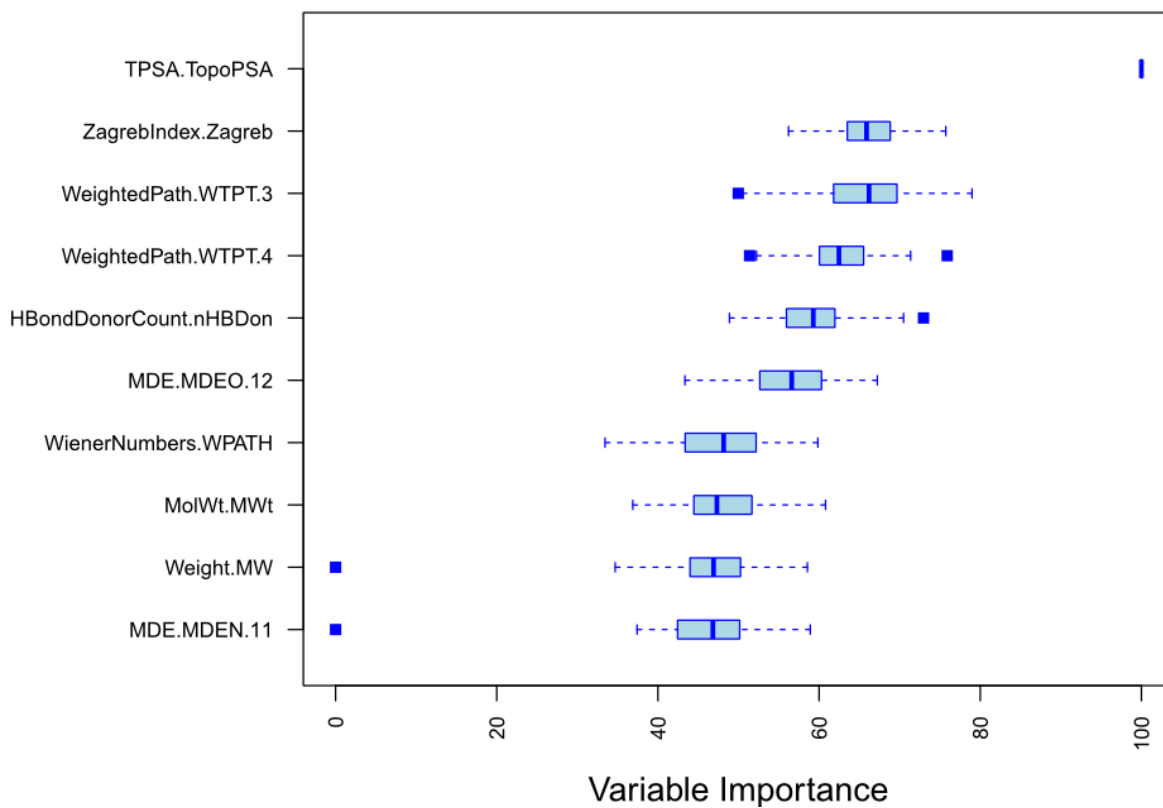


Figure S5. The most important descriptors in the RF model.

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.