

# Solvation Enthalpies and Free Energies for Organic Solvents through a Dense Neural Network: a Generalized-Born Approach

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## Supporting Information

### Content

Part 1. ESE- $\Delta$ H-DNN Dense Neural Network buildup.....	p. 2
56 initial input vector components.....	p. 2
56×40 dimensionality reduction linear transformation.....	p. 2
ESE- $\Delta$ H-DNN weights and biases.....	p. 9
Part 2. Solvents.....	p.11
Part 3. Predicted and reference solvation free energies and solvation enthalpies.....	p. 14
Training and validation sets.....	p. 14
Testing set.....	p. 109
Solvation free energies of nonpolar solvents from MNSol database .....	p. 133

## Part 1.

### ESE-ΔH-DNN Dense Neural Network buildup

#### 56 initial vector components:

- (1) the number of atoms in the solute molecule  $N$ ;
- (2) the molecular volume of the solute  $V = \sum_I V_I$ ;
- (3) the total surface area of the solute  $S = \sum_I S_I$ ;
- (4) atomic surface areas  $S_H$  summed over all hydrogen atoms.
- (5) atomic surface areas  $S_C$  summed over all carbon atoms.
- (6) atomic surface areas  $S_N$  summed over all nitrogen atoms.
- (7) atomic surface areas  $S_O$  summed over all oxygen atoms.
- (8) atomic surface areas  $S_F$  summed over all fluorine atoms.
- (9) atomic surface areas  $S_S$  summed over all sulfur atoms.
- (10) atomic surface areas  $S_{Cl}$  summed over all chlorine atoms.
- (11) atomic surface areas  $S_{Br}$  summed over all bromine atoms.
- (12) atomic surface areas  $S_I$  summed over all iodine atoms.
- (13) Born-type self-term  $E_1^{\text{Born}}(\text{H}) = \sum_{I \in \text{H}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{H}} Q_I^2/R_I$  for the hydrogen atoms.
- (14) Born-type self-term  $E_1^{\text{Born}}(\text{C}) = \sum_{I \in \text{C}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{C}} Q_I^2/R_I$  for the carbon atoms.
- (15) Born-type self-term  $E_1^{\text{Born}}(\text{N}) = \sum_{I \in \text{N}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{N}} Q_I^2/R_I$  for the nitrogen atoms.
- (16) Born-type self-term  $E_1^{\text{Born}}(\text{O}) = \sum_{I \in \text{O}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{O}} Q_I^2/R_I$  for the oxygen atoms.
- (17) Born-type self-term  $E_1^{\text{Born}}(\text{F}) = \sum_{I \in \text{F}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{F}} Q_I^2/R_I$  for the fluorine atoms.
- (18) Born-type self-term  $E_1^{\text{Born}}(\text{S}) = \sum_{I \in \text{S}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{S}} Q_I^2/R_I$  for the sulfur atoms.
- (19) Born-type self-term  $E_1^{\text{Born}}(\text{Cl}) = \sum_{I \in \text{Cl}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{Cl}} Q_I^2/R_I$  for the chlorine atoms.
- (20) Born-type self-term  $E_1^{\text{Born}}(\text{Br}) = \sum_{I \in \text{Br}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{Br}} Q_I^2/R_I$  for the bromine atoms.
- (21) Born-type self-term  $E_1^{\text{Born}}(\text{I}) = \sum_{I \in \text{I}} E_I^{\text{self}} = (1-1/\epsilon) \sum_{I \in \text{I}} Q_I^2/R_I$  for the iodine atoms.
- (22–51)  $\epsilon$ -dependent Born-type pair terms by elements:  $E_2^{\text{Born}}(L_1, L_2) = (1-1/\epsilon) \sum_{I \in L_1} \sum_{J \in L_2} Q_I Q_J / f_{IJ}$
- (22)  $L_1 = \text{H}; L_2 = \text{H}$ ; (23)  $L_1 = \text{C}; L_2 = \text{C}$ ; (24)  $L_1 = \text{C}; L_2 = \text{H}$ ; (25)  $L_1 = \text{N}; L_2 = \text{N}$ ; (26)  $L_1 = \text{N}; L_2 = \text{H}$ ;
- (27)  $L_1 = \text{N}; L_2 = \text{C}$ ; (28)  $L_1 = \text{O}; L_2 = \text{O}$ ; (29)  $L_1 = \text{O}; L_2 = \text{H}$ ; (30)  $L_1 = \text{O}; L_2 = \text{C}$ ; (31)  $L_1 = \text{O}; L_2 = \text{N}$ ; (32)  $L_1 = \text{F}; L_2 = \text{F}$ ; (33)  $L_1 = \text{F}; L_2 = \text{H}$ ; (34)  $L_1 = \text{F}; L_2 = \text{C}$ ; (35)  $L_1 = \text{F}; L_2 = \text{O}$ ; (36)  $L_1 = \text{S}; L_2 = \text{H}$ ; (37)  $L_1 = \text{S}; L_2 = \text{C}$ ;
- (38)  $L_1 = \text{S}; L_2 = \text{N}$ ; (39)  $L_1 = \text{S}; L_2 = \text{O}$ ; (40)  $L_1 = \text{Cl}; L_2 = \text{H}$ ; (41)  $L_1 = \text{Cl}; L_2 = \text{C}$ ; (42)  $L_1 = \text{Cl}; L_2 = \text{N}$ ; (43)  $L_1 = \text{Cl}; L_2 = \text{O}$ ; (44)  $L_1 = \text{Cl}; L_2 = \text{F}$ ; (45)  $L_1 = \text{Br}; L_2 = \text{H}$ ; (46)  $L_1 = \text{Br}; L_2 = \text{C}$ ; (47)  $L_1 = \text{Br}; L_2 = \text{N}$ ; (48)  $L_1 = \text{Br}; L_2 = \text{O}$ ; (49)  $L_1 = \text{Br}; L_2 = \text{Cl}$ ; (50)  $L_1 = \text{I}; L_2 = \text{H}$ ; (51)  $L_1 = \text{I}; L_2 = \text{C}$ ; (52) the dielectric constant  $\epsilon$  of the solvent;
- (53) the boiling point (BP) of the solvent;
- (54) the number of non-hydrogen atoms in the solvent.
- (55) solvent molar volume
- (56) the number of hydrogen-bond centers (donors+acceptors) the solvent molecule.

## 56×40 dimensionality reduction linear transformation:

T(:,1)=(/0.09337227587594887,-0.49829156719600254,0.6527360642081965,0.5166673951728387, &  
0.21147264090841517,-0.009280139758097428,0.009494049077085296,-0.016140681139341584, &  
-0.002871806427014465,-0.027772914225193332,-0.00024916477391602514,-0.0027712027657820866, &  
-0.00010897973268475372,-0.0001018888849489973,6.8436264549301375e-6,-3.0463352061710564e-5, &  
3.83396809125153e-6,8.936094590647957e-6,1.8877513096477973e-7,-1.0602405698078808e-7, &  
1.135974822033371e-8,-0.0001320034514781062,-0.00010823561000312842,0.0003192263088840168, &  
3.094670638638721e-7,-1.7085506126025877e-6,-5.667831438224897e-6,-8.119818213242392e-6, &  
4.139311548571071e-5,-1.9222452594652975e-5,7.839261769408722e-7,2.1459517880202063e-6, &  
-4.952412259967905e-7,-2.2624948200388646e-6,1.033014487870376e-7,6.429672573560111e-8, &  
-1.6937678586752522e-7,-1.887660214048171e-9,-2.3998716147714953e-7,-2.4237648053121234e-7, &  
8.461810785813431e-8,2.986638517802197e-9,7.82782903792243e-9,-1.8803954404686034e-8, &  
1.7202479453953667e-7,-1.4774882740050493e-7,-9.076014202701343e-11,2.2148986325496114e-10, &  
2.6359913860003636e-10,-3.155903502169648e-8,3.16450755987928e-8,0.0006041264687010754, &  
-0.05426837885744268,-0.002597208361657829,-0.03287026848648374,-7.614403556159392e-5/)  
T(:,2)=(/0.005729390919285093,0.02553639612101577,0.039816227201971116,0.04445254431675691, &  
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6.813292943163019e-7,1.5549550255001945e-6,-1.9539653796690987e-8,8.29429922175484e-8, &  
2.0203681989022494e-9,2.6281887470759276e-6,-5.929809000806197e-6,1.1315824789436906e-5, &  
7.427026584564126e-7,-1.4730976890673715e-5,3.9155073439945216e-7,2.645070898774242e-6, &  
-1.2070335505599475e-5,-2.6213910309412834e-6,1.3737005099182832e-6,3.9359457507842455e-7, &  
-4.0790323232794466e-8,-3.756552071664549e-7,-2.7294705660143028e-8,1.338038541250139e-7, &  
-1.1732076486398463e-7,1.8799717458675767e-9,-1.3845514748024364e-8,3.552143901074437e-8, &  
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-1.517366334039348e-7,1.319110779304363e-7,-2.4889794675796936e-10,1.2900933764656049e-9, &  
-1.286289480744381e-10,-7.880959892115577e-9,7.675086581331551e-9,0.02128270882794523, &  
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T(:,3)=(/0.0017709431055195895,-0.0009885715694299027,-0.008760027368521106,0.009353311180943642, &  
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-0.0001077571588640074,-6.588445864813672e-5,-1.657459047054706e-5,-5.5443301493591144e-5, &  
1.4458247200318498e-6,3.315893432646863e-6,-1.5824850420958555e-7,-1.9472235618897305e-8, &  
1.497244132644394e-9,-6.712658443302772e-5,-3.8887011563321185e-5,0.00014380109150702048, &  
-1.1598733543835024e-6,-1.2889894803633537e-5,1.0429112868521118e-6,-6.383239285511819e-6, &  
5.466817347248382e-5,-1.1274527492503445e-5,-1.7037852721380245e-6,1.2492089777124569e-6, &  
4.1625134455386583e-7,-1.0429802369189915e-6,-6.414346827847825e-8,-1.6974825370510901e-7, &  
2.4829156457480359e-7,1.2475539901514275e-9,3.669962381510147e-7,2.5361944563622817e-7, &  
-1.9566416184489276e-7,1.0027609646803414e-8,9.382393067916803e-9,-4.06963418964129e-9, &  
-5.010698381617367e-9,3.50891045545749e-10,-2.32710951288652e-10,4.724848856474344e-10, &  
-8.119821409788814e-11,-8.59525960831319e-9,7.49997519953635e-9,0.5422604263968461, &  
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T(:,4)=(/-0.03454315629402467,0.28491342026292427,0.25987074584649716,-0.5714337758352552, &  
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-0.0007999584311703792,0.7186959950757259,0.01768117240173559,0.008365820997657139, &  
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-1.5252276372307093e-5,-3.36180334435182525e-5,-6.644107045802696e-6,-1.021809908267047e-7, &  
-8.823980465865456e-9,0.00013409340102438054,0.00010356068425076646,-0.00033798540133579463, &  
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-2.1710935067106668e-5,2.28184163815775e-5,1.757981216339399e-6,-8.456940385285104e-6, &  
1.4446133632835887e-6,8.952545057926819e-6,-5.314457770492457e-7,3.9617583590822826e-8, &  
-1.2948806688755726e-7,-8.565468580252939e-9,-8.479380832867613e-8,1.1218316524533709e-5, &  
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4.149865587404939e-9,3.905063507459346e-8,-3.849425082915899e-8,-0.011546636255049094, &  
0.018367373371733105,-0.0004953728844677898,-0.01863019751032095,-0.0002738344413058227/)  
T(:,5)=(/-0.0019889885926893777,0.19001512448780505,0.02318362805564449,-0.4894818085479515, &  
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-8.800822295312524e-5,0.00012719363716031913,-2.011390585366887e-5,-0.00021030134785997038, &  
-1.4241227860963192e-5,-3.2076539522142724e-5,7.148994209208894e-6,2.6941045561048013e-7, &  
-1.8012732537385923e-8,0.00020541321995091438,-0.000519163220636973, &  
-2.146663742312525e-6,-1.2696461289167371e-5,2.4269126607278905e-5,-5.1143263903688055e-5, &  
0.0001700760259252109,1.776085225928809e-5,-1.8378066539552947e-6,-7.852521170615296e-6, &  
3.305889882737633e-6,9.93480703424868e-6,-7.72269700406533e-7,-2.1237776874750708e-7, &  
1.352879083153444e-7,-2.638119906792588e-8,2.9658289030017347e-7,-1.2625239973701089e-5, &  
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T(:,6)=(/-0.0015568148003152814,0.003246438141199185,0.014887349202966246,-0.0211634614361031, &  
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-0.0016814564313419877,0.009804126122504473,0.0033524653104991015,-0.00028065190027474747, &  
4.133386917693716e-5,4.8384336979277113e-5,-7.187122936698499e-6,-4.08503786590767e-6, &  
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1.0957963841400306e-5,-1.2313168872527436e-5,-3.563172916354511e-6,1.9043566198845377e-8, &  
1.7034422965951803e-9,9.849280100083543e-7,-3.2876189591360633e-7,3.1787514121368157e-7, &  
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-1.0594932079451332e-11,-2.4849905941199192e-8,2.6258923242521394e-8,0.8392597424441651, &  
-0.33788238700003753,0.000659845992234496,0.42320711807013284,-0.004646426859243949/)  
T(:,7)=(/-0.0009523123420589127,-0.015925919821975797,0.20665119646558527,-0.04998602908692116, &  
0.5166449737982539,-0.04766426199398466,0.8107251656067829,0.1271985184317419, &  
0.006276237472459895,-0.00943955815137546,-0.017884624549195538,-0.008224495543905763, &  
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-3.5648983683829353e-5,-0.00011068506174794762,3.1319061381614284e-6,2.1495629271999808e-7, &  
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0.0007855414208539151,-0.00011979780183613276,-3.860606894706604e-6,-2.3990580253678184e-5, &  
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-4.799482405310265e-7,4.522301714617806e-7,-1.5523913910405136e-9,2.3622020689060035e-9, &  
2.7883709935299796e-9,-1.162306714267953e-7,1.21615830373775e-7,-0.02635076684018062, &  
0.024363045713325,-0.0015063581082853108,-0.021998403352800212,0.0007296551096189286/)  
T(:,8)=(/0.00011813229681619674,0.060796547335414494,0.12585320819006443,-0.10434896768267257, &

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-0.00022571004650998014,-0.0006022417327355512,2.7656158680935186e-6,-2.293315572941257e-6, &  
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-5.480256709362517e-7,5.184894680026242e-6,-1.1617140156180175e-5,4.740362485233852e-5, &  
0.00026366392161319816,3.306519679662173e-5,3.877757834632955e-6,-0.0001387848166879813, &  
2.560649569853997e-5,0.00010679956856280876,-7.57920233999778e-6,5.388082429669715e-7, &  
-4.2593370467093823e-7,-2.355898353194243e-9,6.168791456077455e-7,-4.938584939342382e-6, &  
2.1339772377632776e-6,3.4423375807946764e-8,1.367194614412465e-7,6.660356117170245e-7, &  
3.815402490186613e-6,-3.4720913723994466e-6,8.744923599050896e-10,-2.841803361025124e-9, &  
8.391410393977729e-9,4.876585545375408e-7,-4.925141517690313e-7,0.0038810831391423595, &  
0.007918952413442225,0.0002384464663045976,-0.01382445785788303,-0.000339050243423645/) &  
T(:,9)=(/-0.0402004953624545,0.15669176982719904,0.10759671924373301,-0.17091599248883016, &  
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T(:,20)=(/0.002477813090713008, 0.00015565893565635074, -0.000554983622313213, -0.0006974247527052329, &  
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3.550118649298106e-5, -0.30670419980041486, -0.24568175960601352, 0.7090062527798304, &  
0.002349864355619918, 0.024517306263039742, 0.010068047300439063, -0.014956791107680008, &  
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0.0008330583855169257, -5.078004531542168e-6, 7.517799946654818e-5, 6.52167283701222e-5, &  
4.251280201190052e-5, -2.7890313513545978e-5, 2.2109160212174724e-7, -7.70256514074599e-6, &  
5.0318010692467034e-8, -0.00011494439720217453, 0.00012077652947211677, 3.991054494219601e-5, &  
-0.00011618083607872931, 0.0023547999056054234, 8.698804188629584e-5, -0.005525779081630696/))  
T(:,21)=(/0.008301426474950569, -0.0011730330889315062, 0.0005519296922457604, -0.0010526522496508886, &  
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-9.295223456180629e-5, -7.441275433250914e-5, -9.105464831121167e-6, 7.707864911269729e-5, &  
0.00031060167862486277, 0.1420064483349759, -0.005628145402550803, 0.008990729745197497, &  
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1.4122381559845577e-5, -0.03659925374909467, -0.03067585744867596, 0.11053982758783175, &  
-0.0005188426112152471, 0.003977004892563259, -0.006035346739298295, 0.0022369562453873463, &  
0.00993225785461607, -0.04828561367006265, 0.003017878971678172, -0.131534335541272, &  
-0.028618643578783822, -0.12165719011808619, 0.008242925919794019, -0.0016466127435745578, &  
0.00176427491189362, 1.4532140146233183e-6, 0.0032774389733669167, 0.0013274133241790676, &  
0.00015235164006161225, -1.723977086821385e-5, -1.6841957972289823e-5, -0.0007767622526995177, &  
0.0003249457059721901, -0.0001561499807021841, 2.670528551662026e-7, -6.754335107651438e-7, &  
-8.352345106547803e-6, -4.649495810155231e-5, 4.749138327564259e-5, 4.007593485830975e-6, &  
9.514482022909005e-6, -0.00014639179633438223, 2.0200032924750697e-5, -0.000329699093926226616/))  
T(:,22)=(/0.00495499345123659, -0.0005058305441283974, 0.00030984145916211544, -0.0005890502055112797, &  
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-0.14538576041142542, -0.552886172686876, 0.043459414588391795, -0.27749918655488487, &

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-0.14003211105989163,0.6663365306110917,-0.055283657182743064,-0.027369000109549707, &  
-0.001161156287862404,0.005513658134602277,-0.002683117601577392,0.00021967193478520923, &  
-9.061813745776824e-5,-2.2083174364551547e-5,-0.00040341897296809943,0.008411434088921213, &  
-0.007387741701230855,-8.78674932599372e-5,-0.00020047331673838718,-0.00012371620941776528, &  
0.004403900679897531,-0.0038804226471777555,7.040050448911852e-7,-9.050183710799794e-6, &  
-1.1503175508979931e-6,0.0004322917344308441,-0.0004388608938639846,1.4211257567533074e-5, &  
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T(:,23)=(/-0.0005729513780334651,-0.0003875411553434763,0.00031261885268791026, &  
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8.64705953515654e-5,5.038105093087016e-6,7.490790060548665e-8,1.1522972087800633e-5, &  
1.192310307331369e-5,-0.1922433642852156,0.533038997794592,0.029089435750524025, &  
0.04032812013563436,0.00880708170627037,0.06047879148291052,0.0002506190448591239, &  
0.0031385276057461775,0.00012218169584689298,0.0797847412128741,-0.6284544583299587, &  
-0.10308112418738011,0.001327396876714293,-0.023961419281961813,0.15622308037990354, &  
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0.011460815820474793,0.014497554734143032,-0.01966143454289166,-0.005423121849851516, &  
0.0106704504779598,-0.010653433847459214,6.67759169792471e-5,-0.009259427198434374, &  
-0.00027346727241903097,0.0014482325730513198,2.5463091404810787e-5,-0.000356967037652253, &  
-0.00012815461174970702,-0.004765018107074957,0.004323033469341655,-3.6215593737784094e-6, &  
-1.8494412220169352e-5,-2.9001478421612875e-6,-0.0004071593688329112,0.00041874222948308157, &  
3.9274475954839004e-6,5.685466589112386e-6,-0.000137553431135929,-1.6920087580373174e-6, &  
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T(:,24)=(/0.0012181598589159936,-0.00025306205488958113,0.00020967753920316459, &  
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-0.000136056326441809987,-3.2048721543544635e-5,-5.685823594015045e-5,-4.708316726461827e-5, &  
-2.8779132869421327e-5,-0.18062407236217692,-0.15337135721942446,-0.1831572312795374, &  
0.047844327583190675,-0.009350197967068596,-0.02586230917943677,-0.004658427749805433, &  
-0.0010261664560826667,-0.00011483137180595682,0.16567735524378577,-0.1111671398977245, &  
0.10217512483414123,-0.06848980042415953,-0.13881798321129735,0.8165239846058052, &  
0.20580245328555816,-0.07147374172802047,-0.3158122016059411,-0.13614116271680313, &  
-0.008868305823115636,0.0014013156427619673,0.01672645805649985,-0.0016149263124833647, &  
-0.004679959615246682,0.004688044821997066,-4.0271594852464786e-5,0.003869097176027054, &  
0.009437455956843617,-0.007938210873430022,-0.0004415509146328848,-0.00021439215612005706, &  
2.2990247804343487e-5,0.0019163428070267784,-0.0017568530971799605,3.0444950576083103e-6, &  
-3.985776844012998e-6,7.972422613368272e-7,0.0004042608715642399,-0.0004102370597515528, &  
-9.974455653749793e-6,1.9053427171816787e-6,-8.158776808604514e-5,2.668504114811432e-6, &  
-6.551717131633548e-5(/)  
T(:,25)=(/-0.0016720653653871326,0.000388069279465783,-0.0003513206112070713, &  
0.00027178465602891604,0.0001880904738841999,-5.837502836653771e-6,0.00019666695802546136, &  
8.86191972447457e-5,3.805179465952485e-5,0.00011246448940859217,0.00010394691042204844, &  
5.749327655289639e-5,0.42636067215309176,-0.28819985744029464,-0.17889712088551926, &  
0.35036480801148395,-0.0021750589210046724,-0.036492865189212416,0.012595015898060669, &  
0.0015487384623546832,1.5595569192096426e-5,-0.26017588523441454,-0.12334539243816678, &  
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-0.47930783374363006,0.4623633918389175,0.06714909094944889,-0.025568037421614946, &  
-0.013289525125242606,-0.028366962378648605,0.041783293693811695,0.008217629903409204, &  
0.007100128749448058,-0.007532202384502205,8.804931495843466e-6,-0.008150804743844288, &  
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0.00044281530369530924,-0.0030702203407311176,0.0025712613091375394,9.03781835996045e-6, &  
7.36424261802812e-5,3.961749795498945e-6,-0.00012427880196613908,0.00010424852368668627, &  
5.380415907443444e-7,9.84610399620713e-7,-3.7335215208577915e-5,1.932497379242694e-6, &  
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T(:,26)=(/0.000511550250539972,-6.443873810661491e-5,6.020999923217347e-5,-5.749358454170308e-5, &  
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6.140432876828526e-6,-5.2656733104230796e-5,-8.604849685431661e-5,-4.940642449612843e-5, &  
-0.6307506974295622,-0.057507277879450674,0.19868990922133625,0.602947510399084, &  
-0.04086836553819853,-0.012993533862475669,-0.06340741086626603,-0.014282453719149685, &  
-0.0006610408163834625,-0.04546005461064624,0.22795324782507798,-0.10340630316469007, &  
0.009769236966749861,-0.1500765618381042,-0.09533482281028083,-0.17202346276980496, &  
0.12825841348237127,-0.02559624686238479,0.11998163839367455,-0.014776127678824214, &  
0.05090675005808576,-0.022275579654547354,-0.011742401392879407,0.027415733967286266, &  
-0.028321592826275246,-0.0001011201986446234,-0.03130867319042719,0.11891725664802336, &  
-0.10518696049988752,-0.00011668312527827875,-0.0006317022158414836,-0.0010237441718771421, &  
0.02411372079867179,-0.021458835262679405,-1.426225043735881e-5,3.624134813439402e-5, &  
-2.122109914233272e-5,0.0021383290781410032,-0.002188519598464029,6.679218037304257e-7, &  
7.130955286920502e-6,0.0002044298814989138,7.310774138435082e-7,-0.0003397598207335689(/)  
T(:,27)=(/0.001195821399779047,-0.00023675467058064585,0.00017526061764497255, &  
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-0.00024457725494759683,-2.8000827756615648e-5,-3.0514482985741966e-5,-7.241962540061195e-6, &  
-9.545147526723963e-6,-0.020021236060739907,-0.30348506529938324,0.3275288092402862, &  
0.09507758974609695,-0.07031486894282653,-0.0682992224460527,0.05176231042676115, &  
0.014739254784078509,-1.488502258444914e-5,0.31619951809785796,-0.38947707437498275, &  
-0.15877707246036078,0.023344754112791268,0.4047288426811454,-0.20448416924442286, &  
0.22503899326129265,0.20370678866021727,-0.19732501282901685,-0.12273170431855152, &  
-0.09389116199671621,-0.032112557612640785,0.3456235291240982,-0.02001330654646196, &  
-0.02347569921942378,0.02353072533122045,0.00010832990109712465,0.015178003728216507, &  
-0.09819187744848296,0.08838153207067369,0.0002380041686638021,-0.0006267864772886052, &  
0.001855600153323568,-0.023770101720246434,0.020634189286103603,-1.5215519806764346e-5, &  
-9.110800927932916e-5,1.9962587139181888e-5,0.00017945439587936998,-0.00017137902529207256, &  
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6.739207240840511e-5(/)  
T(:,28)=(/-0.0006678477302466992,0.0001353259101406117,-0.00010887077349615105, &  
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0.00010964903348828827,1.971710872965098e-5,1.7211402056680617e-5,1.522979047782186e-6, &  
3.9683891107175145e-6,0.011679344367781199,0.08873125934900686,0.4752811857835807, &  
0.038191144624328474,0.014911557369945469,0.02593590376812692,-0.05137908011305713, &  
-0.009985812949628303,-7.743768959833641e-5,-0.38996639396912014,0.17123101467626378, &  
-0.0325249102633664,0.008424885765027144,0.39362674596190933,0.22597116310682708, &  
0.02627308472478622,-0.07072811990697386,0.09278090155846677,-0.542459412364838, &  
0.04318166226139546,0.036261382494014206,-0.20151145777353754,0.010448125868071494, &  
0.03056643474218877,-0.031127134787876484,0.00021644721987211664,-0.030748756344294203, &  
0.09546818470833901,-0.08697753946857853,0.0003616711630336684,0.00039113940203794806, &  
-0.0015505162814457411,0.016535931522906982,-0.01462087178003397,-3.2978001692324654e-5, &  
7.168470668017251e-5,-2.4714687931980066e-5,0.00018476010126625624,-0.00021645214842480034, &  
-2.0571162782233483e-6,1.855580949520195e-6,-5.011643947178167e-5,4.120267888328527e-7, &  
-5.093006011601137e-5(/)  
T(:,29)=(/0.00010793054657515972,-3.9509316250115766e-5,2.334351580702033e-5, &  
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5.040209774804106e-5, -7.163354218177894e-6, 1.043806042901385e-6, 3.2596816742207598e-6, &  
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0.15994602615873893, 0.07100685286470992, 0.004432742981985649, 0.007294221502108317, &  
0.004391511990652977, -8.285776615707396e-5, 0.13123995485048656, -0.0363840604707778, &  
0.022286801962966535, -0.32552682210969874, 0.36984978962499904, 0.19738938657919122, &  
-0.4695686960941071, -0.2085021890469192, -0.1696822146650382, 0.4988575553562489, &  
0.06376676012534958, -0.03046981567126071, -0.15298722959208527, 0.02691399271567344, &  
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-0.014920929437651147, 0.01300735176035261, 0.00040828988140502866, 0.0008287101194894148, &  
-0.00024752368099340656, -0.006921976678900894, 0.0060247242390212286, -3.42326816572582e-5, &  
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2.0999697546734628e-6, -1.1286649243100362e-6, 1.81130769573842e-5, -3.4767531969029375e-7, &  
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T(:,30)=(/-0.0009515801919338457, 0.00014233789116982622, -9.8516919124161e-5, 0.00012619279093592552, &  
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T(:,31)=(/1.913237869789052e-5, -2.7721327417374542e-5, 2.413469390306286e-5, -1.607944656853368e-6, &  
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-0.02468407316251156, 0.022117094104475078, 9.38450280606751e-6, 1.7193895817248678e-5, &  
-1.983172258030624e-5, -0.0006377265573744953, 0.0006584048899084611, 8.347531096977723e-7, &  
-9.12878825792135e-7, 4.074502065010144e-5, -6.731371544714537e-7, -5.945162545263963e-5/)  
T(:,32)=(/-0.0003312131738800237, 3.503036286774171e-5, -2.5236045957543334e-5, &  
5.21613833713468e-5, 3.3518235179698962e-6, 1.5008845441330043e-5, -1.344122641298249e-5, &  
-2.861559181901196e-5, 1.45800346447331619e-5, 2.3219705449468416e-5, -1.3723833215955552e-5, &  
-2.8684336898137826e-6, -0.13112971772953247, 0.054385920514584865, 0.02990594942775972, &  
-0.05359139788082834, -0.2800389250872552, 0.04302160205709797, 0.2532098833319143, &  
-0.04097659990082072, -0.0007717397750479822, -0.09223574543263917, 0.0302897584752106, &  
-0.03630801349420868, 0.2709069505975344, -0.05895930542041161, 0.028643303530839395, &  
-0.3301515309066709, -0.2198051329107388, -0.1110752793949472, -0.12622993577775343, &  
-0.108221172674848657, 0.2533453534022167, 0.11314472991626245, -0.05464711857978541, &  
0.08657661865547006, -0.08643273168173433, -8.273004728019239e-5, -0.11077509559399894, &  
-0.4800190366755881, 4.4567681788488256, 0.0003462249989853311, 0.003695431885815628, &  
-0.0009866263400515017, 0.06678113695040201, -0.05954822683264546, -3.247999810860157e-5, &  
0.00017013616807051105, 4.74636795506977e-5, 0.002319018643596342, -0.0023897754603973923, &  
-6.652998457701287e-8, -1.6772477172410927e-6, 3.111548014384205e-5, 8.270662190945632e-7, &  
-8.708835720817923e-5/)  
T(:,33)=(/-7.903755943573334e-5, 1.7196027036374336e-5, -1.5438293806209935e-5, &  
1.1502176836797902e-5, 7.888912716896553e-6, -1.0723431974368736e-5, 7.78005811030404e-6, &  
-2.9752299709542207e-5, -2.5487005172188797e-5, 6.731948044412618e-6, -7.345800762972139e-6, &  
3.8097442209023845e-7, -0.02386957806887413, -0.019071568769348634, -0.005398648303922791, &  
0.06920813336280292, -0.1278734048889107, 0.004870631282849248, 0.060537169109156526, &  
-0.0310615614851021826, -0.0002304404807928302, -0.188232161120102, -0.010937498556556777, &  
-0.08197323195740333, -0.27587474403816875, -0.08086879268807591, -0.045423654148447026, &  
0.15645016255459465, 0.03052274985765374, 0.06252420331139366, -0.015031067677149193, &  
0.04507567719185839, 0.35099788522320474, -0.04517802439253574, -0.1329944986143539, &  
-0.4445542478821999, 0.4573310490645149, 0.0004985381521509791, 0.48522282735767164, &  
-0.1122770885963814, 0.1108599629265151, 0.00012133599237971592, 0.00021527304196278935, &  
-0.004379056285385037, 0.05094190999875767, -0.04503864695000809, -1.1062498679340846e-5, &  
7.546651658785317e-5, -4.563742397039748e-6, 0.0007107571379474506, -0.000743183233873043, &  
8.947880054954727e-8, -8.89701412987165e-7, 2.0682238391939167e-5, 6.20105998772047e-7, &  
-2.0710517235469905e-5/)  
T(:,34)=(/0.0003156073576673405, -3.0105807973890752e-5, 1.4422222229854536e-5, &  
-4.420639383214e-5, -5.422443819977683e-6, 1.9479675153248048e-6, -6.025689050592842e-6, &  
-6.875219243797407e-5, 6.912702387262747e-6, -7.860556547654599e-6, 3.401221796651734e-5, &  
8.110512091088511e-6, 0.1006685111577735, -0.09518810455054416, -0.012407448712962607, &  
-0.06198110459533519, -0.4220811276105006, 0.08240510693899628, -0.13074449858616824, &  
0.12142914688542869, 0.001372999916886171, 0.0661484837873242, -0.12129595407273482, &  
-0.02329776828335868, 0.3084783674565992, 0.08553130798861262, 0.01208095051267001, &  
0.022347420693777972, 0.02908551504350712, -0.059978349442833825, 0.1656030822066054, &  
-0.056458995179763605, 0.5515442434520259, -0.2890286707594714, -0.11367461728376424, &  
0.03537312960998823, -0.03913650080763492, -0.00014114269905072955, -0.09860871229259378, &  
0.2513715533470465, -0.22875386373926226, -0.0008069913191665959, -0.0007885624863792212, &  
-0.005340465246919442, -0.20346086658134674, 0.1790855704463869, 7.295941878183751e-5, &  
-0.00019932013079394535, 0.0001165325234776817, -0.004295057063990242, 0.004412380028023211, &  
4.401165888540115e-7, -7.047161976192484e-8, -3.343135058786473e-7, -1.0713670221818017e-7, &  
1.7739828134466507e-5/)  
T(:,35)=(/-0.000304483131099427, 3.536431931541712e-5, -1.534269606808377e-5, 3.801047899548078e-5, &  
-6.1933840029842625e-6, 1.016038827754798e-6, 1.7413068710566094e-5, 5.155253808021092e-6, &  
7.96564801339313e-6, 4.445084957190774e-6, 3.7227317747459706e-5, 5.906942434874933e-8, &  
-0.05576533609744191, 0.0069927998866550645, -0.1122116385735739, -0.047525335634292596, &  
-0.09662407940166876, 0.02535884915704698, -0.01564162317234805, 0.1904015186403596, &  
0.00027363814756244803, 0.15137935320240467, -0.05814499535540561, 0.02686438262266785, &  
-0.5891447509910518, -0.15861106019412222, -0.2118969961049733, -0.24766985760501, &  
-0.08146930770260168, -0.12544758446665616, -0.4525477208156993, -0.03440689361961921, &  
0.07498352324603222, -0.024651016754195704, 0.007249638959843062, 0.06715109948306634, &  
-0.06985594714854272, 0.00014523991179919867, -0.09344777047145916, 0.0305150602398373, &  
-0.023690887956299006, 0.0010803426337476422, -0.0007042672635501727, 0.0004327920336449865, &  
-0.3141612536406657, -0.2775798246338768, 8.825886961649572e-5, -0.0002745236264494036, &  
0.00012740564758403363, -0.0009987560105117462, 0.0018856342311007796, -3.374714573345372e-7, &  
-1.24540029722865e-6, 3.358892124815174e-5, 1.1199654287863403e-6, -6.470647876832825e-5/)  
T(:,36)=(/-0.00017970789015562554, -7.655098823029628e-6, 1.7926864721395878e-5, &

1.1579079215966678e-5,1.079270004719872e-5,5.862146676154206e-6,1.2012992984702127e-5, &  
-7.523210798762109e-6,4.99628531795008e-6,-1.432059043539098e-6,-4.5166662630686636e-5, &  
3.4713349962198e-6,0.040359830812534137,-0.05414388275250635,-0.07909902711536829, &  
-0.075903274455686033,-0.1588040436811879,0.03844487727441782,-0.08333341649954397, &  
-0.34088660028277307,0.0029021863984981574,0.14385918802202644,-0.14308396136302823, &  
-0.006165069911281892,-0.20282184517382318,-0.03800344588071437,-0.13890601540939645, &  
-0.11156514231017102,-0.02034193933153408,-0.11595725882765351,-0.1745662306799636, &  
-0.029568808450224554,0.1437879895051734,-0.13760363077226279,0.009428224243007701, &  
0.04368285319399361,-0.04909647396310577,0.00020708740877365057,-0.13653904852478677, &  
0.16450086968404606,-0.15521069294446593,-0.0002831176317099962,-0.00278689853210419, &  
0.0014134122379007486,0.560342708656849,-0.4948247813821832,-0.00011857148687436296, &  
0.0003582379316672415,-0.00011874679874934822,-0.00920492058664087,0.009495305636910444, &  
3.146099970541272e-7,-3.674562042976781e-7,2.9728609506646242e-5,-5.053695432688521e-7, &  
-3.852735441339794e-5/)  
T(:,37)=(/-2.7485971647581538e-5,-8.47713567250225e-6,8.022520222570961e-6,2.4603811737032758e-6, &  
-2.3711375519067263e-6,-8.555223476322412e-7,-1.4874466144249572e-5,3.0373297046675298e-5, &  
-1.6514858090302357e-5,1.0037899271543158e-7,1.406422873042539e-6,1.410489858605069e-6, &  
-0.06260463563985313,-0.14705700118054432,-0.005131698358227033,-0.05027945710086293, &  
0.41996760261936095,-0.11220905389952572,-0.01384311698471493,-0.0011915052300672752, &  
0.0009031422409939475,-0.2533695792179778,-0.24939945475934672,-0.25367349532453715, &  
0.014405904318785596,-0.10104694537053574,-0.12882787606318974,-0.0003748340426448088, &  
-0.14777214687585893,-0.14632008809196528,0.03132503087018532,0.14640448385265506, &  
-1.6983919678351067,-0.08759186697382679,-0.387579054735157,0.3210157205335293, &  
-0.32070941517603385,-0.00010575179649978947,0.3230442271845505,0.03908614440099635, &  
0.015145424070705679,-0.0008989779877454406,-0.004043714560874434,-0.020313799375162117, &  
0.010415279628937478,-0.0030803509239844505,-1.3760524999835276e-5,2.6317706684147383e-5, &  
-0.0003283140520159275,-0.002851439437739453,0.0029168294500845045,-1.6162757043858278e-7, &  
-8.202250249556009e-7,2.3358321012412198e-5,-5.468716034184862e-8,-3.7289990190203515e-5/)  
T(:,38)=(/3.833772903636449e-6,1.20142288289401e-5,-1.0976116180246363e-5,-1.4841766259683276e-6, &  
8.205021657933278e-6,4.469975656938582e-6,1.9599736176866595e-5,-1.1628432438114378e-5, &  
-7.6375124569953e-6,1.8721296744120878e-6,-2.6593759995050415e-6,-1.2006089975626475e-7, &  
0.09932671573451467,0.18107258538646903,-0.005398462185096192,0.04195450403865039, &  
-0.05845659395325253,-0.003100037677832025,-0.004583277017847646,-0.026716264872668066, &  
-0.00028213378072233265,0.38428316520634964,0.30829866089954633,0.34784456318880524, &  
-0.04037064575647991,0.1413926873789123,0.15058105690134183,-0.05339225410373247, &  
0.18711729786579884,0.15478020669359022,-0.00091617645062917,0.061381110027868856, &  
0.19766585511641266,0.25758657603612567,-0.2641995462587524,0.21505103167726602, &  
-0.24497108790936356,-0.0008371353237970809,0.4300224603873815,-0.006675170681487014, &  
-0.0319741924027125,0.0006179967793520091,0.006831809601532318,0.005246628527073249, &  
0.04367679619671167,-0.04235851809730912,2.999368249948322e-5,-2.4794137189900357e-5, &  
8.036308509393056e-5,0.000813896076122346,-0.0008252147285008546,5.279077167075208e-8, &  
5.910313490287145e-7,-1.7631395830164376e-5,-2.915772051304e-7,3.7208913768516094e-5/)  
T(:,39)=(/-1.4491133918177343e-6,-5.2340112217129766e-6,5.9982793715917834e-6, &  
-8.922687732117069e-7,-3.4351796197145655e-6,-1.6148580606775233e-6,-5.860628741275677e-6, &  
-3.7262975884121305e-5,-9.518757398481709e-6,-2.001593169703015e-6,-9.4186911521042e-7, &  
-5.139398915327817e-7,-0.030071626492594233,-0.05339266094649242,-0.00017794994810210017, &  
-0.007484298495161723,-0.5053257514760959,0.05937689511277652,0.013461036503825739, &  
-0.002623776401807613,0.00030598338735276023,-0.11030531162222537,-0.09047302504779998, &  
-0.10128871741896786,0.006298828220559886,-0.043347388893109,-0.045964461339926, &  
0.03442841670714962,-0.045159865775655894,-0.03726049497172812,0.026999307094478286, &  
0.25936914127538463,-0.293796424172684,-0.09286463556303398,0.454509084015505, &  
0.20269879459371687,-0.2153535116713423,-0.00026820223706338156,0.48745145961015185, &  
-0.022019832630712152,-0.03650020433337939,0.0005049353738359099,-0.0033365956376491396, &  
0.03615076435081065,-0.011152262054443583,0.003220582795195527,-2.2067934553068698e-5, &  
-5.466630263329395e-5,0.0005231870058786898,-0.0007093623806548547,0.0007680426122606745, &  
5.1143713750145814e-8,-3.611094626376765e-7,-7.252779009314647e-7,8.375800194353189e-7, &  
-1.376901463145952e-5/)  
T(:,40)=(/2.219988467729626e-5,-2.5842584632704913e-6,1.4362838850138602e-6,-3.379984620408517e-6, &  
-1.0080400981436206e-8,-6.533407163131698e-7,3.893371671102838e-7,9.606632167124316e-6, &  
-4.51424153777054e-6,-6.017141846227858e-7,-1.250539465322134e-7,3.9886932799179963e-7, &  
0.008202592572264975,0.0050608289312384135,-0.0009290498644566616,0.0022536497913907016, &  
0.347134216651725,-0.0030282980607055643,-0.050003729576889595,0.002499358143454775, &  
0.002251763182538163,0.017068473762305525,0.010495174992151482,0.014465784980439, &  
0.0007008061857383639,0.007985392577008858,0.006033722626672108,0.007945906255283283, &  
0.013415960256247583,0.009631339078795792,0.002580998105310456,-0.4356686166895233, &  
0.39207514772660035,0.027355500043657693,0.6560304038479658,0.07486013612782286, &  
-0.09132129099828715,-0.0008154247199918278,0.1891002208630351,0.1228908787851467, &  
0.15951302020576846,-0.009037997997911856,-0.028870261245856312,-0.09909329922407493, &  
0.008861661796645316,-0.0020105789486974425,3.5518392473418756e-5,-0.00022138757761967255, &  
-0.00033961138916989555,-0.007061350172554491,0.007273063693667376,9.436567807719065e-8, &  
4.408141008466204e-8,-4.795957375597348e-6,1.5302871352040892e-7,4.441901578555729e-6/)



## ESE-ΔH-DNN weights and biases

### Scaling factors:

InputFeaturesNormalized(1:40) = InputFeatures(1:40)/NormDivisor(1:40)

where

NormDivisor=(/576.7324,252.2554,299.4501,213.7513,147.3593,161.9005,133.4692,161.8137,118.4256,55.15629,27.25552,61.66297,45.4025,10.17672,3.77464,3.164353,0.3063627,0.2580394,0.1280841,0.2516345,0.08408053,0.05513559,0.09719245,0.03858832,0.03587171,0.03404153,0.03776263,0.0324423,0.02984245,0.02417255,0.01739873,0.02066965,0.01361684,0.01128766,0.01248827,0.007994611,0.008824335,0.003645347,0.003735296,0.003194017/)

### 1st hidden layer. Activation function: ReLU.

#### Weights and biases:

Weights1(:,1) = (/ -0.156825379,0.0019160799,0.069854781,-0.125201389,-0.100511976, &  
-0.110685833,-0.0674225911,0.0896153525,-0.107168496,-0.0477325879,-0.0617494397, &  
0.051074408,0.0460720994,-0.0421234556,0.0437229834,-0.000594177167,-0.00449120533, &  
-0.115741044,0.00389032927,-0.0700752139,0.00292804907,-0.0744445398,0.134500146, &  
-0.151096627,0.0178595912,0.0461424328,0.123189889,-0.133650601,0.138021529, &  
-0.0343164429,-0.00918805227,0.0101330047,-0.181553885,0.0725992322,-0.301558018, &  
-0.0593016893,-0.235070989,0.198554069,-0.205050707,-0.0120945815/)  
Weights1(:,2) = (/0.0931303278,0.0157496389,0.272039473,0.00349099236,-0.0779805705, &  
-0.229976237,0.0695830658,0.0986839011,0.0124443183,0.0188744515,0.00689016702, &  
-0.0225582011,-0.0201525856,-0.0479001552,-0.26189056,-0.0708864182,0.0230377316, &  
0.0593471192,-0.052065596,0.0353423506,-0.0316474363,-0.126665518,-0.017336553, &  
-0.229638785,0.214161634,-0.0286052935,0.0624164455,0.0431417823,-0.0764230937, &  
-0.010214244,-0.0658034682,-0.0317560956,-0.0265324861,-0.0415087901,-0.0126722325, &  
0.000386475935,-0.00315172016,0.0370351933,0.0197645016,-0.0505414829/)  
Weights1(:,3) = (/0.226421073,-0.0578859411,0.0557772815,0.0902804285,0.201322854, &  
0.01601151,0.0301406551,-0.146512762,0.0604760498,0.0615520403,0.00733299321, &  
-0.0722894296,-0.0419517905,-0.00548528088,-0.00324785546,0.0523592308,0.00452644425, &  
0.0139443325,-0.0419939719,-0.0520588718,-0.0145313255,0.0464773811,-0.0645226911, &  
-0.0165512301,-0.060069941,0.0685025677,-0.151423857,-0.0894213542,-0.00445200223, &  
0.0678521246,0.11877241,0.0926896632,-0.0148019148,0.0138534987,0.0773761496, &  
0.0403524116,0.0164146796,-0.0405125245,0.0362823419,0.0276434701/)  
Weights1(:,4) = (/0.154017031,-0.00804845802,-0.0127534382,0.214928269,0.0598925576, &  
-0.0684137642,-0.119347461,-0.141677037,0.0435307957,0.00300609507,0.0139358025, &  
-0.0760014504,-0.0311613549,0.211778283,0.00219314755,0.0143928928,-0.0315457471, &  
0.0446137264,-0.00664698565,-0.0730244741,0.0354605801,0.0597208627,0.0301000867, &  
0.0450255126,0.034401726,-0.0655986965,-0.147469923,0.000210197832,-0.0405491516, &  
0.0624284521,0.0643732622,0.118879698,0.0417991988,-0.0441981666,0.0838819817, &  
-0.0255691633,0.00633673882,-0.0344770774,0.00191128626,0.0117794424/)  
Weights1(:,5) = (/0.00118315057,-0.0806992128,0.16650705,0.117625393,0.156663537, &  
-0.090756312,0.0764820427,-0.164633676,-0.126658306,0.0191740673,0.0125851259, &  
-0.0336294882,0.0678285211,0.0460376926,0.0049025137,0.067405723,-0.0121317692, &  
0.103188083,-0.00462537073,-0.0859491378,0.0194912814,-0.00429020217,-0.0764318854, &  
0.0422907285,0.16243425,0.0782717094,0.0189628955,0.171989858,-0.181574896, &  
-0.0887901857,-0.0539111085,0.0945706218,0.0368103385,-0.0173731856,-0.16101177, &  
-0.17179428,0.138738394,-0.125407308,0.0681274086,-0.0215887092/)  
Weights1(:,6) = (/0.0132952677,-0.015357621,0.0408360064,-0.171470091,-0.148208469, &  
-0.0530267507,-0.17867665,0.109924123,0.0189135447,0.0078885965,0.0784024894, &  
0.131685659,0.0608001612,0.140735716,0.263273776,-0.0437909029,-0.0777559131, &  
0.093379207,-0.135679677,0.199047282,0.0938134864,-0.0211077835,0.0477827862, &  
-0.0265866164,-0.0406072214,-0.0472331233,0.151421934,0.150898427,-0.0100969672, &  
0.0484683961,-0.0555212572,-0.0488949232,0.0889135003,-0.0481915772,0.0486415625, &  
-0.0947004035,-0.0933340117,-0.0229582991,-0.0139010614,0.0269023702/)  
Weights1(:,7) = (/0.182168692,-0.0160227418,-0.276249766,-0.000718546042,0.0393285528, &  
-0.211306155,0.0368194617,0.0272435341,-0.0807759017,0.00595929567,-0.0161920115, &  
0.152257949,-0.115406662,0.0461911671,-0.0046445271,-0.044535283,0.000184189543, &  
0.218443885,0.0670775697,0.122272193,0.00695879199,0.0125635797,0.0106647741, &  
-0.0539717972,-0.0497929566,-0.120226793,-0.0593480095,0.018432254,-0.0624738932, &  
-0.0218968093,-0.126204357,-0.058638338,0.0508405454,-0.0738826618,-0.0172513612, &  
-0.109943166,-0.0307496078,0.106614903,-0.0784051195,-0.0188516025/)  
Weights1(:,8) = (/ -0.0736252964,-0.0182543099,0.0814961717,-0.126780838,-0.119529255, &  
-0.03254712,0.00841676537,0.110102676,0.0330766179,0.0069979853,-0.0508664474, &  
0.111406885,-0.0695727617,-0.0771447271,-0.145379558,-0.0831056163,-0.0242091715, &  
-0.162877753,-0.0251379702,0.0818175077,0.000891298929,-0.086887233,-0.253595829, &  
-0.0679680482,0.14427422,-0.0656072423,-0.0633566976,0.000397746626,-0.102357984, &  
0.0349663086,-0.22503753,-0.0332688652,-0.0733634531,0.105532505,-0.113619104, &  
-0.0228384547,-0.0247003511,-0.247603551,-0.0148508018,-0.043584127/)  
Weights1(:,9) = (/ -0.024309013,0.0469595678,0.254065871,-0.0937732905,0.0238087978, &  
-0.00916019455,0.112331502,-0.159712002,-0.0134802526,-0.00175926776,0.0131785376, &  
-0.067019403,0.0463996567,0.0884615332,0.163711682,-0.0530786254,-0.03894113, &  
0.196567252,-0.15928492,0.172774523,0.0698338673,-0.00166263583,0.183148801, &  
-0.133169577,-0.273965269,-0.00412102323,0.018250959,-0.0983221829,-0.136170313, &

```

-0.0433513969,-0.202896073,-0.243094593,0.0824320838,0.0272639617,-0.200358108, &
-0.122996099,-0.152027443,0.0711795911,0.0068176426,0.0268481988/)
Weights1(:,10) = (/0.183023855,-0.0501271412,-0.0948785692,-0.0165550578,0.0935359523, &
0.0389382131,-0.0588917211,-0.00491408259,0.00950607378,-0.0233115349,0.00140440883, &
0.0192680769,-0.0999226272,0.110306464,0.0800796151,0.0061010723,-0.0979844108, &
0.0389576443,-0.00305768079,0.098794058,0.0463401079,0.0633716285,0.136773452, &
-0.0318506919,0.0622029603,-0.044922214,-0.0077781789,0.0427699126,-0.0103327166, &
0.033545129,0.0137666771,-0.0505545959,0.095025517,0.013822848,0.00852657203, &
-0.0323102325,-0.0254799519,0.0309236422,-0.0275271237,-0.020351233/)
Weights1(:,11) = (/ -0.167838782,0.0769115761,0.176912591,-0.0760519728,-0.0500479117, &
-0.145203456,-0.0148397302,0.156455025,-0.00397071848,0.0541098826,0.163887471, &
0.0952276215,0.112206817,-0.092001237,0.0130361356,-0.0251902919,-0.00830002781, &
-0.110550955,-0.153056413,0.0318482406,-0.01358632,0.00166949944,-0.000825508614, &
-0.185534149,0.0740450174,-0.152147561,-0.0425733067,0.00553350616,0.0150337052, &
-0.00720076449,0.00726700108,0.0956512094,0.0311975367,0.0405700132,-0.0407647789, &
0.020732753,0.0666626692,-0.00502904272,0.104302205,-0.0495381765/)
Weights1(:,12) = (/ -0.070943214,-0.0269117728,-0.0963889137,-0.0213283952,-0.137038499, &
0.0641780794,-0.131602019,0.133408681,-0.070537366,0.00196628994,0.0293861832, &
-0.00439235428,-0.0934438109,0.0934110582,-0.154064,0.108145133,0.0708460137, &
0.0497922935,0.181199476,0.230475038,-0.0718090311,0.0452575311,0.347778469, &
0.069552362,-0.147907868,-0.0285328664,0.183119714,-0.0685315281,-0.136887461, &
-0.140732139,-0.211474583,-0.123962671,0.0419767611,-0.104209222,-0.171068579, &
-0.147762597,-0.089562729,0.193938181,0.0496374927,0.0907230452/)
Weights1(:,13) = (/ -0.0330922045,-0.0654459521,-0.00509227114,-0.0732140914,0.0690715238, &
-0.036447566,0.150787458,-0.0986096561,0.0285828821,0.0326030813,0.0462539941, &
-0.00922461785,-0.0558567494,0.0599204898,-0.0915315226,0.03814172,0.0281352978, &
0.0853262469,0.0174050722,0.190063715,-0.000467285223,0.11160858,0.096909292, &
0.0920799375,-0.373444051,0.00936833024,-0.00283041992,-0.129908264,0.080728516, &
-0.0418145061,-0.189954907,-0.161899894,0.00868174061,0.126020133,-0.0557740889, &
-0.0475032292,0.00707723526,0.154144615,-0.0184641331,0.0413458534/)
Weights1(:,14) = (/0.127067238,0.00376508385,-0.0710095465,0.0576625168,-0.0149312923, &
-0.142056838,-0.200648338,0.0358220376,0.0575450733,-0.0258713737,0.0788574666, &
0.0946774408,0.0433468409,-0.0823789835,0.0200350843,-0.0294683464,0.0104367062, &
0.0416037068,-0.0670306608,0.0239005182,-0.00959334429,-0.175098211,0.00957337767, &
0.219100997,-0.109148517,-0.0247029755,0.00948051643,-0.0847632587,-0.0554314628, &
-0.0396345109,0.101719096,-0.036645133,-0.0109330444,-0.0425491855,0.147872478, &
0.0962989032,-0.0299560353,0.0160797834,0.015949741,-0.0316692404/)

Biases1 = (/0.206974998,0.14000988,0.0113803409,0.0970930532,0.051087983,-0.0115636773, &
0.0371399708,0.256153047,-0.0653399155,0.105076984,0.0253675282,0.0831663981, &
0.0308380071,-0.0459716842/)

```

2nd hidden layer. Activation function: ReLU.

Weights and biases:

```

Weights2(:,1) = (/0.262830496,-0.0461477675,-0.0284341685,-0.0802103281,-0.233236134, &
0.256013632,-0.283147216,-0.00496042473,-0.173511356,0.0904367119,0.169160321, &
0.442582369,-0.263982892,-0.268859237/)
Weights2(:,2) = (/ -0.251591653,0.227325514,0.082785666,0.193907619,0.237001866, &
-0.223528802,0.225804672,-0.278657109,0.314146221,0.171499819,-0.226863295, &
-0.242718339,0.266670763,0.114146963/)
Weights2(:,3) = (/ -0.279294759,0.339638233,-0.133253217,0.026075745,0.289522946, &
-0.344102591,0.190928593,-0.313225687,0.393442184,0.225093946,-0.311185896, &
-0.362891912,0.249246284,0.0571389198/)
Weights2(:,4) = (/ -0.244414955,0.183955103,0.17579776,0.230394647,0.228985429, &
-0.205633745,0.23180826,-0.237231568,0.279145479,0.147595152,-0.206236795, &
-0.229772583,0.250364602,0.151205733/)
Weights2(:,5) = (/ -0.238413841,0.326048583,-0.121985748,0.0413215011,0.256481439, &
-0.25982222,0.175369963,-0.256146967,0.380477786,0.141123384,-0.114585124, &
-0.349462658,0.2635957,0.21659413/)
Weights2(:,6) = (/ -0.215584785,-0.000229698227,0.388232678,0.315973878,0.146102875, &
-0.069549866,0.229672194,-0.097782664,0.129143387,0.0177793819,-0.14986816, &
-0.151996791,0.158295214,0.258411556/)

Biases2 = (/0.101692781,0.0916541964,0.102310918,0.0855584592,0.0829352513,0.0721694753/)

```

Output layer. Activation function: linear.

Weights and biases:

```

Weights3(:,1) = (/9.70144939,-10.3960075,-3.65312481,-12.7001696,-2.50226402,-17.8584595/)
Weights3(:,2) = (/19.6721649,-17.7004223,-23.3846436,-15.794961,-21.1929512,-7.9532218/)

Biases3 = (/ -0.4108,-2.906/)

```

## Part 2 – Solvents

**Table S1.** Solvents and their properties (for using in ESE-ΔH-DNN program)

Solvent	Synonyms	Dielectric constant	Boiling point, °C	Number of heavy atoms	Molar volume, mL/mol	number of hydrogen-bond centers
ethyl acetate	ethylacetate, ethyl-acetate	5.9867	77.1	6	97.8	2
methyl acetate		6.6	56.9	5	79.9	2
fluorooctane	fluorooctane, 1-fluorooctane	3.89	142.6	9	163.2	1
butyl acetate	butylacetate, butyl-acetate	4.9941	126.1	8	132.1	2
butylbenzene		2.36	182.9	10	156.2	0
tert-butylbenzene	tbutylbenzene, t-butylbenzene	2.38	168.9	10	155.6	0
sec-butylbenzene	secbutylbenzene	2.34	172.9	10	156.4	0
isopropylbenzene	cumene	2.38	151.9	9	140.3	0
isopropyltoluene	o-cymene, ortho-cymene	2.23	178.0	10	150.8	0
propyl acetate		6.3	101.6	7	115.1	2
pentyl acetate		4.75	146.9	9	148.8	2
hexyl acetate		4.42	169.9	10	165.6	2
isobutyl acetate		5.6	116.9	8	132.8	2
ethyl butanoate		5.1	120.9	8	132.2	2
ethyl hexanoate		4.57	168.1	10	165.6	2
ethylbenzene		2.4339	136.2	8	123.0	0
m-xylene	meta-xylene, 1,3-dimethylbenzene	2.4	139.2	8	123.5	0
o-xylene	ortho-xylene, 1,2-dimethylbenzene	2.57	143.9	8	121.2	0
p-xylene	para-xylene, 1,4-dimethylbenzene	2.3	138.2	8	123.9	0
xylene	dimethylbenzene	2.39	138.4	8	123.5	0
toluene		2.3741	110.7	7	106.3	0
benzene		2.2706	81.0	6	88.9	0
N,N-dimethylformamide	dimethyl_formamide, dimethylformamide, dimethyl-formamide	37.219	152.9	5	77.0	1
N,N-dimethylacetamide	N,N-dimethyl_acetamide, dimethylacetamide, dimethyl_acetamide, dimethyl-acetamide	37.7807	165.1	6	92.5	1
N-methyl-2-pyrrolidone		32.2	202.1	7	96.2	1
N,N-diethylacetamide		31.33	184.1	8	127.4	1
N,N-dibutylformamide		18.4	200.0	11	182.0	1
N-methyl_formamide	N-methylformamide, methylformamide	181.5619	182.6	4	58.9	2
N-methyl_acetamide	N-methylacetamide, methylacetamide	178.9	205.1	5	77.3	2
formamide	N-formamide	111.0	210.0	3	39.8	2
chloroform	trichloromethane	4.7113	61.2	4	80.2	0
tetrachloroethene	tetrachloroethylene	2.50	121.1	6	101.7	0
chlorohexane	1-chlorohexane	5.95	134.6	7	137.4	0
decalin		2.23	190.1	10	154.8	0
tetralin	tetraline, benzocyclohexane, tetrahydronaphthalene, baccin, tetranap	2.77	206.9	10	135.7	0
dichloromethane	methylenechloride, methylene_chloride, methylene-chloride	8.93	39.9	3	64.1	0
1-chlorobutane		9.6	76.9	5	104.5	0
carbon tetrachloride	carbontet, tetrachloromethane	2.228	76.7	5	97.1	0
dichloroethane	1,2-dichloroethane	10.125	83.6	4	78.8	0
bromoethane		9.01	38.4	3	74.1	0
methylene iodide		5.3	150.0	3	80.6	0
hexadecyl iodide	hexadecyliodide, iodohectadecane	3.53	400.0	17	314.6	0
dibromomethane		7.8	96.9	3	69.6	0
fluorobenzene		5.42	84.9	7	93.9	1
chlorobenzene		5.6968	131.8	7	101.8	0
bromobenzene		5.3954	156.0	7	105.1	0
iodobenzene		4.547	188.2	7	111.4	0
perfluorobenzene	hexafluorobenzene	2.029	80.2	12	115.8	6
acetone		21.4	56.2	4	73.7	1
2-butanone	butanone, methyl_ethyl_ketone, methylethylketone, MEK	18.2457	79.9	5	89.6	1
ortho-nitrotoluene	onitrotoluene, o-nitrotoluene	27.4	222.9	10	118.0	2
2-pentanone		15.45	101.9	6	106.6	1
3-pentanone		17.3	101.9	6	105.7	1
2-hexanone		14.56	126.9	7	124.1	1
2-heptanone		11.95	149.9	8	140.8	1

4-methyl-2-pentanone	4methyl2pentanone, MIBK, methyl_isobutyl_ketone, isobutyl_methyl_ketone	12.8871	115.9	7	125.1	1
cyclohexanone		15.6186	154.9	7	104.2	1
acetophenone		17.44	201.9	9	117.3	1
cyclopentanone		14.45	129.9	6	89.1	1
2-methylcyclohexanone		14.0	118.5	8	121.5	1
benzonitrile		25.592	190.9	8	103.1	1
tributylphosphate	tributyl_phosphate, tributyl- phosphate	8.1781	293.0	17	272.9	4
propylene carbonate		64.9	240.1	7	85.0	3
carbon disulfide	carbondsulfide	2.6105	46.1	3	59.8	0
triethylamine		2.3832	89.1	7	139.1	1
ethoxybenzene		4.1797	170.2	9	126.6	1
2-methylpyridine	2methylpyridine	9.9533	128.9	7	99.1	1
dimethylpyridine		7.33	142.0	8	116.3	1
benzyl ether		3.86	298.1	15	189.9	1
phenyl ether	phenyl-ether, phenylether	3.9	259.1	13	159.1	1
3-methylphenol	m-cresol, mcresol	11.5	202.1	8	104.4	1
acetic acid	aceticacid	6.2528	118.1	4	57.1	2
bromoform	tribromomethane	4.4	148.9	4	89.4	0
bromooctane	1-bromooctane, octyl_bromide	5.0	201.0	9	173.7	0
nitroethane		28.2896	114.5	5	71.2	2
benzyl alcohol	benzylalcohol	12.4569	204.9	8	103.6	1
butyronitrile		20.7	117.9	5	86.9	1
aniline		6.8882	183.9	7	91.5	1
nitromethane		36.5623	101.0	4	53.7	2
nitrobenzene		34.8091	210.9	9	102.3	2
dimethylsulfoxide	DMSO	46.826	189.9	4	70.9	1
propionitrile		27.7	96.9	4	69.6	1
acetonitrile	MeCN	35.6881	81.7	3	52.5	1
ethyl benzoate		6.0	211.9	11	143.4	2
sulfolane	sulfolan, tetramethylene_sulfone	44.0	284.9	7	95.4	2
pyridine		12.9776	115.4	6	80.5	1
dimethyl carbonate	dimethyl-carbonate	3.17	90.4	6	84.0	3
diethyl carbonate	diethyl-carbonate	3.1	126.5	8	121.0	3
methanol		32.613	64.7	2	40.5	1
ethanol		24.852	78.4	3	58.4	1
1-propanol	propanol	20.5237	97.2	4	74.8	1
1-butanol	butanol, n-butanol	17.3323	117.5	5	91.5	1
isobutanol	2-methylpropanol	16.68	107.7	5	92.5	1
1-pentanol	pentanol, n-pentanol, amyl_alcohol, amyl-alcohol	15.13	137.9	6	108.3	1
1-hexanol	hexanol	12.5102	156.9	7	125.6	1
1-heptanol	heptanol	11.321	174.9	8	141.9	1
1-decanol	decanol, n-decanol	7.5305	231.9	11	191.0	1
1-dodecanol	dodecanol, n-dodecanol	6.5	261.1	13	224.3	1
2-propanol	isopropanol	19.2645	82.4	4	76.4	1
2-butanol	sec-butanol, secbutanol	15.9436	100.0	5	91.8	1
2-methyl-1-propanol		16.7766	107.7	5	92.5	1
tert-butanol	t-butanol, tbutanol	10.9	82.4	5	94.9	1
1-octanol	octanol	9.8629	194.9	9	157.4	1
nonanol	1-nonanol	8.83	212.0	10	174.4	1
2-methyl-2-butanol		5.82	102.0	6	108.2	1
ethylene glycol	ethylene-glycol	37.0	197.4	4	55.7	2
propylene glycol	propylene-glycol	32.0	188.2	5	73.4	2
2-heptanol		9.21	158.9	8	142.8	1
4-heptanol		6.17	154.9	8	142.6	1
4-octanol		5.12	175.0	9	159.7	1
allyl_alcoholallyl- alcohol		21.0	96.9	4	68.1	1
2, 2, 2-trifluoroethanol	trifluoroethanol	8.55	74.9	6	71.8	4
pentane	n-pentane	1.8371	36.1	5	115.2	0
hexane	n-hexane	1.8819	68.8	6	130.7	0
heptane	n-heptane	1.9113	98.4	7	146.6	0
octane	n-octane	1.9406	125.6	8	163.4	0
nonane	n-nonane	1.9605	150.7	9	179.6	0
decane	n-decane	1.9846	174.1	10	196.0	0
dibromoethane	1,2-dibromoethane	4.75	131.0	4	86.1	0
undecane		1.991	194.9	11	212.1	0
dodecane		2.006	215.9	12	228.6	0
2, 2, 4-trimethylpentane	isooctane	1.9358	99.2	8	165.1	0
hexadecane	n-hexadecane	2.0402	280.9	16	294.1	0

methylcyclohexane	cyclohexylmethane, mchx	2.02	100.9	7	128.4	0
tetradecane		2.03	249.9	14	260.2	0
pentadecane		2.0333	266.9	15	277.7	0
cyclooctane		2.12	148.9	8	134.9	0
cyclohexane		2.0165	80.8	6	108.7	0
methoxyethanol	2-methoxyethanol, methyl-cellosolve, methyl_cellosolve, methylcellosolve, EGME	17.2	124.4	5	78.9	2
ethoxyethanol	2-ethoxyethanol, cellosolve, ethylcellosolve, ethyl_cellosolve, ethyl-cellosolve, oxitol	5.3	135.1	6	96.9	2
2-butoxyethanol	butylcellosolve, butyl_cellosolve, butyl-cellosolve	5.3	171.1	8	131.0	2
diethylene glycol	diethylene-glycol	31.7	245.9	7	95.1	3
triethylene glycol	triethylene-glycol	23.07	266.9	10	133.5	4
diethyl ether	diethylether, diethyl-ether	4.24	34.6	5	103.9	1
dibutyl ether	dibutylether, dibutyl-ether	3.0473	141.9	9	169.1	1
diisopropyl ether	diisopropylether, diisopropyl-ether	3.38	68.2	7	140.7	1
methyl tert-butyl ether	methyl-tert-butyl-ether	4.5	55.1	6	119.0	1
dipropyl ether	dipropyl-ether	3.39	89.9	7	146.0	1
tetrahydrofuran	THF	7.4257	65.9	5	81.3	1
1,4-dioxane	dioxane	2.25	101.2	6	85.2	2
bis-2-ethoxyethyl ether		5.7	185.1	11	179.1	3
tetrahydropyran		5.68	87.9	6	97.9	1
2, 5-dimethyltetrahydrofuran		3.05	92.9	7	120.2	1
anisole		4.45	153.9	8	109.2	1
tridecane		2.02	233.9	13	243.9	0
1,2-dichlorobenzene	odichlorobenzene, o-dichlorobenzene, ortho-dichlorobenzene	7.5	180.6	8	112.6	0
benzotrifluoride		9.4	101.9	10	121.9	3
1,3-dioxolane		7.34	74.6	5	70.0	2
1,3, 5-trimethylbenzene	trimethylbenzene, mesitylene	2.4	164.7	9	139.6	0
2-methyltetrahydrofuran		6.97	78.9	6	100.7	1

### Part 3 – Predicted and reference solvation free energies and solvation enthalpies

**Table S2.** Predicted and reference solvation free energies and solvation enthalpies in kcal/mol – training and validation sets. The entries that belong to the validation set are marked by an asterisk in the rightmost column

Solute	Solute SMILES	Solvent	$\Delta^{\text{ref}}G_{\text{solv}}^{\circ}$	$\Delta^{\text{pred}}G_{\text{solv}}^{\circ}$	$\Delta^{\text{ref}}H_{\text{solv}}^{\circ}$	$\Delta^{\text{pred}}H_{\text{solv}}^{\circ}$
methane	C	2-butanol		0.38	-1.02	-0.85
ethane	CC	2-butanol		-0.52	-2.85	-2.25
propane	CCC	2-butanol		-1.25	-4.45	-3.38
isobutane	CC(C)C	2-butanol		-1.77	-4.41	-4.21
butane	CCCC	2-butanol		-1.93	-4.76	-4.48
hexane	CCCCCC	2-butanol		-3.44	-6.91	-6.91
heptane	CCCCCCC	2-butanol		-4.17	-8.00	-8.11
nonane	CCCCCCCC	2-butanol		-5.55	-10.18	-10.37
dodecane	CCCCCCCCCCC	2-butanol		-7.60	-13.32	-13.79
hexadecane	CCCCCCCCCCCCCCC	2-butanol		-10.08	-17.70	-17.68
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	2-butanol		-3.94	-7.73	-7.86
cyclohexane	C1CCCCC1	2-butanol		-3.86	-7.23	-7.18
cyclooctane	C1CCCCCCC1	2-butanol		-5.23	-9.59	-9.43
bicyclohexyl	C1CCC(CC1)C2CCCCC2	2-butanol		-7.59	-12.96	-12.45
1-propene	CC=C	2-butanol		-1.61	-4.15	-3.86
cis-2-butene	C/C=C/C	2-butanol		-2.25	-4.75	-4.81
trans-2-butene	C/C=C/C	2-butanol		-2.28	-4.85	-4.88
isobutene	CC(C)=C	2-butanol		-2.10	-4.84	-4.59
methanol	CO	2-butanol		-3.72	-9.15	-8.49
butan-1-ol	CCCCO	2-butanol		-5.66	-12.62	-11.82
decan-1-ol	CCCCCCCCCO	2-butanol		-9.63	-19.14	-18.20
2-butanol	CCC(C)O	2-butanol		-5.34	-11.88	-11.25
chloroform	ClC(Cl)Cl	2-butanol		-4.15	-7.24	-7.84
tetrachloromethane	ClC(Cl)(Cl)Cl	2-butanol		-4.22	-7.30	-8.03
2-chlorobutane	CCC(C)Cl	2-butanol		-3.75	-6.45	-7.05
2-chloro-1-methylpropane	CCC(C)Cl	2-butanol		-3.84	-6.72	-7.19
2-chloro-2-methylbutane	CCC(C)(C)Cl	2-butanol		-3.96	-6.96	-7.27
3-chloro-3-methylpentane	CCC(C)(C)CC	2-butanol		-4.58	-8.19	-8.28
1,2-dichloroethane	ClCCCl	2-butanol		-4.25	-5.92	-7.63
trichloroethene	ClC=C(Cl)Cl	2-butanol		-4.44	-8.30	-8.33
2-methyl-2-bromobutane	CCC(C)(C)Br	2-butanol		-4.22	-7.66	-7.88
2-methyl-2-iodopropane	CC(C)(C)I	2-butanol		-4.17	-7.08	-7.09
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	2-butanol		-7.95	-12.55	-12.80
methyl ethyl ketone	CCC(C)=O	2-butanol		-3.93	-6.57	-6.93
dimethyl ether	COC	2-butanol		-2.12	-4.15	-4.28
methyl tert-butyl ether	COC(C)(C)C	2-butanol		-3.31	-6.63	-6.34
2-methyltetrahydrofuran	CC1CCCO1	2-butanol		-4.06	-7.51	-7.05
1,4-dioxane	C1COCCO1	2-butanol		-4.55	-7.04	-7.96
aniline	Nc1ccccc1	2-butanol		-7.50	-11.47	-13.18
neon	[Ne]	2-butanol		1.88	1.35	1.75
argon	[Ar]	2-butanol		0.91	-0.42	0.12
krypton	[Kr]	2-butanol		0.31	-1.24	-0.62
xenon	[Xe]	2-butanol		-0.69	-2.37	-2.36
hydrogen	[H][H]	2-butanol		1.52	0.86	1.01
deuterium	[H][H]	2-butanol		1.52	0.94	1.01
carbon dioxide	O=C=O	2-butanol		-0.57	-2.21	-2.60
sulfur hexafluoride	F[S](F)(F)(F)F	2-butanol		0.31	-1.93	-1.30
propyl formate	CCCOC=O	2-butanol		-3.89	-6.92	-6.82
methyl acetate	COC(C)=O	2-butanol		-3.59	-5.45	-6.25
propyl acetate	CCCOC(C)=O	2-butanol		-4.51	-7.60	-7.88
propyl propionate	CCCOC(=O)CC	2-butanol		-4.95	-8.54	-8.59
methyl butanoate	CCCC(=O)OC	2-butanol		-4.54	-7.40	-7.88
propyl butanoate	CCCOC(=O)CCC	2-butanol		-5.83	-8.77	-10.18
acetonitrile	CC#N	2-butanol		-4.19	-5.50	-6.61
1-butylamine	CCCCN	2-butanol		-5.27	-10.25	-11.08
1-heptylamine	CCCCCCN	2-butanol		-6.78	-13.62	-13.75
dibutylamine	CCCCNCCCC	2-butanol		-6.42	-13.72	-13.57
triethylamine	CCN(CC)CC	2-butanol		-4.43	-10.02	-9.22
tripropylamine	CCCN(CCC)CCC	2-butanol		-5.98	-11.18	-12.11
benzene	c1ccccc1	2-butanol		-4.06	-6.89	-7.38
chlorobenzene	Clc1ccccc1	2-butanol		-5.28	-8.90	-9.16
acetophenone	CC(=O)c1ccccc1	2-butanol		-7.29	-10.82	-12.01
benzaldehyde	O=Cc1ccccc1	2-butanol		-6.57	-9.45	-10.83
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	2-butanol		-9.82	-17.63	-17.21
dimethyl carbonate	COC(=O)OC	2-butanol		-4.15	-5.98	-7.16
diethyl carbonate	CCOC(=O)OCC	2-butanol		-4.77	-7.85	-8.25
methyl isobutyl ketone	CC(C)CC(C)=O	2-butanol		-5.21	-8.51	-9.18
sebacic acid	OC(=O)CCCCCCCCC(=O)O	2-butanol		-14.33	-28.27	-28.96
2-pyrrolidone	O=C1CCCN1	2-butanol		-8.62	-15.74	-15.87
methane	C	isobutanol		0.46	-1.01	-0.82
ethane	CC	isobutanol		-0.45	-2.91	-2.23
propane	CCC	isobutanol		-1.17	-4.32	-3.36
hexane	CCCCCC	isobutanol		-3.34	-7.15	-6.85
heptane	CCCCCCC	isobutanol		-4.07	-8.17	-8.05
octane	CCCCCCCC	isobutanol		-4.75	-9.33	-9.25
decane	CCCCCCCCC	isobutanol		-6.18	-11.30	-11.47
dodecane	CCCCCCCCCCC	isobutanol		-7.54	-13.82	-13.82

hexadecane	CCCCCCCCCCCCCCC	isobutanol	-10.12	-17.50	-17.93
3-ethylpentane	CCC(CC)CC	isobutanol	-3.78	-8.03	-7.59
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	isobutanol	-3.85	-7.99	-7.81
cyclohexane	C1CCCCC1	isobutanol	-3.90	-7.34	-7.44
cyclooctane	C1CCCCCCC1	isobutanol	-5.29	-9.87	-9.71
ethene	C=C	isobutanol	-0.89	-2.43	-2.88
1-butene	CCC=C	isobutanol	-2.23	-5.19	-4.94
cis-2-butene	C/C=C/C	isobutanol	-2.17	-5.06	-4.80
trans-2-butene	C/C=C/C	isobutanol	-2.21	-5.14	-4.87
isobutene	CC(C)=C	isobutanol	-2.02	-5.03	-4.57
1,3-butadiene	C=CC=C	isobutanol	-2.52	-4.95	-5.31
acetylene	C#C	isobutanol	-1.37	-4.60	-3.72
methanol	CO	isobutanol	-3.66	-8.82	-8.50
butan-1-ol	CCCCO	isobutanol	-5.62	-12.49	-11.90
isobutanol	CC(C)CO	isobutanol	-5.60	-12.14	-11.87
2-methoxyethanol	COCCO	isobutanol	-5.81	-10.19	-12.43
benzene	c1ccccc1	isobutanol	-3.97	-7.25	-7.34
chloroform	ClC(Cl)Cl	isobutanol	-4.07	-7.90	-7.81
tetrachloromethane	ClC(Cl)(Cl)Cl	isobutanol	-4.13	-7.64	-7.99
chloroethane	CCCl	isobutanol	-2.50	-5.26	-5.25
2-chloro-1-methylpropane	CCC(C)Cl	isobutanol	-3.84	-6.90	-7.33
2-chloro-2-methylpropane	CC(C)(C)Cl	isobutanol	-3.28	-6.19	-6.29
2-chloro-2-methylbutane	CCC(C)(C)Cl	isobutanol	-3.96	-7.48	-7.40
2-chloro-2-methylpentane	CCCC(C)(C)Cl	isobutanol	-4.58	-8.68	-8.41
1,2-dichloroethane	ClCCCl	isobutanol	-4.24	-6.93	-7.74
1-bromobutane	CCCCBr	isobutanol	-4.23	-7.81	-8.07
2-methyl-2-bromopropane	CC(C)(C)Br	isobutanol	-3.64	-6.80	-7.05
2-methyl-2-iodopropane	CC(C)(C)I	isobutanol	-4.17	-7.65	-7.21
acetone	CC(C)=O	isobutanol	-3.15	-5.59	-5.77
methyl ethyl ketone	CCC(C)=O	isobutanol	-3.87	-6.59	-6.93
2-methyltetrahydrofuran	CC1CCCO1	isobutanol	-4.12	-7.61	-7.34
1,4-dioxane	C1COCCO1	isobutanol	-4.56	-7.14	-8.14
aniline	Nc1ccccc1	isobutanol	-7.49	-11.55	-13.28
argon	[Ar]	isobutanol	0.96	-0.44	0.15
krypton	[Kr]	isobutanol	0.36	-1.29	-0.65
xenon	[Xe]	isobutanol	-0.63	-2.45	-2.37
radon	[Rn]	isobutanol	-0.83	-2.74	-2.64
hydrogen	[H][H]	isobutanol	1.53	0.88	1.01
nitrogen	N#N	isobutanol	1.00	0.07	0.29
carbon monoxide	C=O	isobutanol	0.79	-0.34	-0.28
carbon dioxide	O=C=O	isobutanol	-0.52	-2.64	-2.64
oxygen	O=O	isobutanol	1.02	-0.42	0.01
carbon tetrafluoride	FC(F)(F)F	isobutanol	0.89	-0.64	-0.62
sulfur hexafluoride	F[S](F)(F)(F)F	isobutanol	0.27	-2.02	-1.53
propyl formate	CCCOC=O	isobutanol	-3.83	-6.73	-6.82
ethyl acetate	CCOC(C)=O	isobutanol	-3.85	-6.79	-6.81
butyl acetate	CCCCOC(C)=O	isobutanol	-5.01	-8.73	-8.84
methyl propionate	CCC(=O)OC	isobutanol	-3.73	-6.67	-6.57
ethyl propionate	CCOC(=O)CC	isobutanol	-4.35	-7.70	-7.65
propyl propionate	CCCOC(=O)CC	isobutanol	-4.87	-8.99	-8.57
methyl butanoate	CCCC(=O)OC	isobutanol	-4.47	-7.79	-7.85
ethyl butanoate	CCCC(=O)OCC	isobutanol	-5.06	-8.37	-8.94
propyl butanoate	CCCOC(=O)CCC	isobutanol	-5.75	-9.04	-10.15
acetonitrile	CC#N	isobutanol	-4.08	-5.69	-6.48
1-butylamine	CCCCN	isobutanol	-5.25	-10.66	-11.19
1-heptylamine	CCCCCCN	isobutanol	-6.78	-14.17	-13.93
dibutylamine	CCCCNCCCC	isobutanol	-6.42	-14.44	-13.75
tripropylamine	CCCN(CCC)CCC	isobutanol	-5.97	-12.00	-12.28
chlorobenzene	Clc1ccccc1	isobutanol	-5.26	-7.98	-9.25
nitromethane	C[N+](=O)[O-]	isobutanol	-4.09	-6.43	-7.66
acetophenone	CC(=O)c1ccccc1	isobutanol	-7.22	-11.22	-11.93
tetramethylsilane	C[Si](C)(C)C	isobutanol	-2.83	-5.50	-5.40
benzaldehyde	O=Cc1ccccc1	isobutanol	-6.52	-9.84	-10.82
acenaphthene	C1Cc2ccccc2c1c23	isobutanol	-8.87	-12.76	-14.78
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	isobutanol	-9.89	-17.92	-17.52
benzoic acid	OC(=O)c1ccccc1	isobutanol	-9.47	-17.36	-17.59
β-pinene	CC1(C)C2CCC(=C)C1C2	isobutanol	-6.24	-10.51	-10.85
dimethyl carbonate	COC(=O)OC	isobutanol	-4.07	-6.81	-7.14
diethyl carbonate	CCOC(=O)OCC	isobutanol	-4.68	-8.14	-8.20
methyl isobutyl ketone	CC(C)CC(C)=O	isobutanol	-5.20	-8.56	-9.28
dimethyl malonate	COC(=O)CC(=O)OC	isobutanol	-6.74	-11.20	-11.37
2-pyrrolidone	O=C1CCCN1	isobutanol	-8.59	-15.93	-15.85
methane	C	1-propanol	0.48	-0.50	-0.81
ethane	CC	1-propanol	-0.40	-2.47	-2.20
propane	CCC	1-propanol	-1.13	-4.45	-3.34
isobutane	CC(C)C	1-propanol	-1.63	-4.97	-4.12
pentane	CCCCC	1-propanol	-2.43	-6.07	-5.38
hexane	CCCCCC	1-propanol	-3.16	-7.15	-6.55
heptane	CCCCCCC	1-propanol	-3.89	-8.07	-7.75
octane	CCCCCCCC	1-propanol	-4.57	-9.19	-8.95
nonane	CCCCCCCCC	1-propanol	-5.30	-10.46	-10.08
decane	CCCCCCCCC	1-propanol	-6.00	-11.32	-11.18
dodecane	CCCCCCCCCCC	1-propanol	-7.36	-13.88	-13.51

hexadecane	CCCCCCCCCCCCCCC	1-propanol	-10.00	-18.05	-17.74
2,3-dimethylbutane	CC(C)C(C)C	1-propanol	-2.78	-6.66	-5.98
3-ethylpentane	CCC(CC)CC	1-propanol	-3.59	-7.99	-7.29
cyclohexane	C1CCCCC1	1-propanol	-3.82	-7.44	-7.37
cyclooctane	C1CCCCCCC1	1-propanol	-5.20	-9.79	-9.64
bicyclohexyl	C1CCC(CC1)C2CCCCC2	1-propanol	-7.63	-13.23	-12.81
methylcyclohexane	CC1CCCCC1	1-propanol	-4.29	-8.08	-8.10
1-propene	CC=C	1-propanol	-1.50	-4.48	-3.83
cis-2-butene	C/C=C/C	1-propanol	-2.14	-5.15	-4.79
trans-2-butene	C/C=C/C	1-propanol	-2.17	-5.11	-4.86
isobutene	CC(C)=C	1-propanol	-1.99	-5.18	-4.56
1-hexene	CCCCC=C	1-propanol	-3.45	-6.96	-6.94
1-heptene	CCCCC=C	1-propanol	-4.15	-8.13	-8.07
methanol	CO	1-propanol	-3.66	-8.96	-8.54
ethanol	CCO	1-propanol	-4.23	-10.09	-9.59
propan-1-ol	CCCO	1-propanol	-4.95	-11.35	-10.81
butan-1-ol	CCCCO	1-propanol	-5.54	-12.47	-11.79
pentan-1-ol	CCCCCO	1-propanol	-6.35	-13.58	-13.18
octan-1-ol	CCCCCCCCO	1-propanol	-8.38	-16.75	-16.40
isopropanol	CC(C)O	1-propanol	-4.62	-10.88	-10.32
3-methyl-1-butanol	CC(C)CCO	1-propanol	-6.19	-13.38	-12.79
2-methyl-2-butanol	CCC(C)(C)O	1-propanol	-5.07	-12.60	-11.08
benzene	c1ccccc1	1-propanol	-4.01	-7.59	-7.50
toluene	Cc1ccccc1	1-propanol	-4.75	-8.60	-8.70
1,2-dimethylbenzene	Cc1ccccc1C	1-propanol	-5.39	-9.50	-9.76
1,3-dimethylbenzene	Cc1cccc(C)c1	1-propanol	-5.36	-9.43	-9.67
1,4-dimethylbenzene	Cc1ccc(C)cc1	1-propanol	-5.36	-9.68	-9.67
tetrachloromethane	ClC(Cl)(Cl)Cl	1-propanol	-4.16	-7.86	-8.10
chloroethane	CCCl	1-propanol	-2.49	-5.62	-5.27
2-chloro-2-methylpropane	CC(C)(C)Cl	1-propanol	-3.33	-6.53	-6.46
2-chloro-2-methylbutane	CCC(C)(C)Cl	1-propanol	-4.02	-7.87	-7.58
3-chloro-3-methylpentane	CCC(C)(C)CC	1-propanol	-4.63	-8.99	-8.58
trichloroethene	ClC=C(Cl)Cl	1-propanol	-4.42	-8.11	-8.49
2-methyl-2-bromobutane	CCC(C)(C)Br	1-propanol	-4.17	-8.50	-7.97
2-methyl-2-iodopropane	CC(C)(C)I	1-propanol	-4.31	-7.98	-7.56
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	1-propanol	-7.99	-13.39	-13.19
acetone	CC(C)=O	1-propanol	-3.33	-5.98	-6.21
methyl ethyl ketone	CCC(C)=O	1-propanol	-3.95	-6.91	-7.14
dimethyl ether	COC	1-propanol	-2.02	-4.37	-4.24
diethyl ether	CCOCC	1-propanol	-3.13	-6.24	-6.04
diisopropyl ether	CC(C)OC(C)C	1-propanol	-4.03	-7.76	-7.75
methyl tert-butyl ether	COC(C)(C)C	1-propanol	-3.32	-6.85	-6.57
methyl tert-amyl ether	CCC(C)(C)OC	1-propanol	-3.84	-8.22	-7.49
tetrahydrofuran	C1CCOC1	1-propanol	-3.64	-6.92	-6.68
tetrahydropyran	C1CCOCC1	1-propanol	-4.25	-8.23	-7.63
1,4-dioxane	C1COCCO1	1-propanol	-4.72	-7.36	-8.53
1,2-dimethoxyethane	COCCOC	1-propanol	-4.71	-8.03	-8.61
1,2-diethoxyethane	CCOCCOCC	1-propanol	-5.63	-9.56	-10.12
diglyme	COCCOCCOC	1-propanol	-7.19	-10.19	-12.69
tetraglyme	COCCOCCOCCOCCOC	1-propanol	-10.71		-19.44
hexaglyme	COCCOCCOCCOCCOCCOCCOC	1-propanol	-13.68		-24.79
15-crown-5	C1COCCOCCOCCOCCO1	1-propanol	-10.44	-16.78	-20.21
18-crown-6	C1COCCOCCOCCOCCOCCOCCO1	1-propanol	-11.80	-20.95	-22.83
aniline	Nc1ccccc1	1-propanol	-7.53	-12.88	-13.41
argon	[Ar]	1-propanol	0.99	-0.40	0.17
xenon	[Xe]	1-propanol	-0.60	-2.30	-2.36
nitrogen	N#N	1-propanol	0.99	0.28	0.23
carbon monoxide	C=O	1-propanol	0.78	-0.41	-0.32
carbon dioxide	O=C=O	1-propanol	-0.68	-2.33	-3.02
oxygen	O=O	1-propanol	1.09	0.12	0.01
ethyl acetate	CCOC(C)=O	1-propanol	-4.03	-7.14	-7.20
ethyl isobutyrate	CCOC(=O)C(C)C	1-propanol	-4.89	-7.91	-8.78
methyl benzoate	COC(=O)c1ccccc1	1-propanol	-7.34	-11.74	-12.15
ethyl benzoate	CCOC(=O)c1ccccc1	1-propanol	-8.03	-12.98	-13.39
propyl benzoate	CCCOC(=O)c1ccccc1	1-propanol	-8.67	-14.01	-14.55
butyl benzoate	CCCCOC(=O)c1ccccc1	1-propanol	-9.51	-14.96	-16.01
ethyl lactate	CCOC(=O)C(C)O	1-propanol	-6.89	-12.19	-14.18
butyronitrile	CCCC#N	1-propanol	-5.41	-7.60	-8.80
chlorobenzene	Clc1ccccc1	1-propanol	-5.24	-9.44	-9.28
4-methylpyridine	Cc1ccncc1	1-propanol	-6.23	-11.19	-10.45
1,3-dichlorobenzene	Clc1cccc(Cl)c1	1-propanol	-6.48	-10.91	-11.10
1,3-dimethoxybenzene	COc1cccc(OC)c1	1-propanol	-7.74	-12.44	-13.13
ethylbenzene	CCc1ccccc1	1-propanol	-5.43	-9.58	-9.74
tetramethylsilane	C[Si](C)(C)C	1-propanol	-2.85	-5.50	-5.49
tetramethylstannane	C[Sn](C)(C)C	1-propanol	-3.85	-7.28	-7.07
1-butylamine	CCCCN	1-propanol	-5.16	-11.19	-11.07
sec-butylamine	CCC(C)N	1-propanol	-4.25	-11.16	-10.07
isobutylamine	CC(C)CN	1-propanol	-4.81	-11.14	-10.71
tert-butylamine	CC(C)(C)N	1-propanol	-4.03	-8.39	-9.98
1-heptylamine	CCCCCCN	1-propanol	-6.76	-14.39	-14.01
triethylamine	CCN(CC)CC	1-propanol	-4.36	-10.61	-9.39
tripropylamine	CCN(CCC)CCC	1-propanol	-5.91	-11.93	-12.28
1,3-diaminopropane	NCCCN	1-propanol	-7.33	-16.61	-16.06



carbon tetrafluoride	FC(F)(F)F	1-propanol	0.98	-0.27	-0.52
succinic acid	OC(=O)CCC(O)=O	1-propanol	-11.39	-22.87	-23.08
adipic acid	OC(=O)CCCCC(O)=O	1-propanol	-12.73	-25.31	-25.84
2,2,2-trifluoroethanol	OCC(F)(F)F	1-propanol	-4.53	-11.55	-11.38
methylformamide	CNC=O	1-propanol	-6.63	-12.24	-12.83
dimethylformamide	CN(C)C=O	1-propanol	-5.67	-10.47	-10.86
anthracene	c1ccc2cc3ccccc3cc2c1	1-propanol	-10.58	-17.29	-17.63
fluoromethane	CF	1-propanol	-0.64	-1.94	-2.17
trimethyl phosphate	CO[P](=O)(OC)OC	1-propanol	-7.50	-9.68	-10.38
tributyl phosphate	CCCCO[P](=O)(OCCCC)OCCCC	1-propanol	-11.66	-19.05	-19.23
acenaphthene	C1Cc2cccc3ccccc1c23	1-propanol	-8.98	-13.86	-15.12
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	1-propanol	-9.89	-17.83	-17.62
benzamide	NC(=O)c1ccccc1	1-propanol	-10.99	-19.49	-19.35
benzoic acid	OC(=O)c1ccccc1	1-propanol	-9.52	-17.87	-17.75
sebacic acid	OC(=O)CCCCCCCCC(O)=O	1-propanol	-14.40	-28.21	-29.32
trifluoromethane	FC(F)F	1-propanol	-0.78	-2.99	-2.49
2-methylpyridine	Cc1ccccc1	1-propanol	-6.26	-11.24	-10.59
3-methylpyridine	Cc1ccncc1	1-propanol	-6.27	-11.15	-10.55
R-fenchone	C[C@H]12CCC(C1)C(C2=O)(C)C	1-propanol	-8.03	-11.16	-13.63
water	O	1-propanol	-4.09	-10.46	-10.27
imidazole	[nH]1ccnc1	1-propanol	-9.20	-17.43	-16.66
xenon	[Xe]	1-pentanol	-0.51	-2.33	-2.37
methane	C	1-pentanol	0.61	-0.60	-0.73
propane	CCC	1-pentanol	-1.03	-4.40	-3.30
butane	CCCC	1-pentanol	-1.72	-5.25	-4.40
isobutane	CC(C)C	1-pentanol	-1.56	-5.02	-4.14
pentane	CCCCC	1-pentanol	-2.47	-6.22	-5.62
hexane	CCCCCC	1-pentanol	-3.25	-7.27	-6.91
heptane	CCCCCCC	1-pentanol	-3.98	-8.42	-8.11
octane	CCCCCCCC	1-pentanol	-4.66	-9.67	-9.29
nonane	CCCCCCCCC	1-pentanol	-5.40	-10.69	-10.43
hexadecane	CCCCCCCCCCCCCCCC	1-pentanol	-10.24	-18.50	-18.38
3-ethylpentane	CCC(CC)CC	1-pentanol	-3.69	-8.11	-7.65
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	1-pentanol	-3.73	-8.07	-7.77
methylcyclopentane	CC1CCCC1	1-pentanol	-3.72	-7.12	-7.36
cyclohexane	C1CCCCC1	1-pentanol	-3.90	-7.53	-7.70
cyclooctane	C1CCCCCCC1	1-pentanol	-5.30	-9.94	-10.00
1-propene	CC=C	1-pentanol	-1.39	-4.42	-3.78
1-butene	CCC=C	1-pentanol	-2.08	-4.68	-4.87
trans-2-butene	C/C=C/C	1-pentanol	-2.06	-5.09	-4.80
isobutene	CC(C)=C	1-pentanol	-1.88	-4.73	-4.51
1,3-butadiene	C=CC=C	1-pentanol	-2.38	-4.90	-5.24
1-hexene	CCCCC=C	1-pentanol	-3.47	-7.93	-7.13
heptan-1-ol	CCCCCCO	1-pentanol	-7.63	-15.92	-15.52
octan-1-ol	CCCCCCCCO	1-pentanol	-8.38	-16.90	-16.59
decan-1-ol	CCCCCCCCCO	1-pentanol	-9.64	-19.32	-18.67
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	1-pentanol	-10.06	-17.88	-18.16
dimethyl ether	COC	1-pentanol	-1.97	-4.22	-4.35
dibutyl ether	CCCCOCCCC	1-pentanol	-5.77	-10.22	-10.66
diisopropyl ether	CC(C)OC(C)C	1-pentanol	-3.74	-7.47	-7.29
methyl tert-butyl ether	COC(C)(C)C	1-pentanol	-3.02	-7.10	-6.12
tetrachloromethane	ClC(Cl)(Cl)Cl	1-pentanol	-3.97	-7.78	-7.88
chloroethane	CCCl	1-pentanol	-2.36	-5.46	-5.19
1-chloropropane	CCCCl	1-pentanol	-3.12	-6.32	-6.36
1-chlorobutane	CCCCCl	1-pentanol	-3.88	-7.52	-7.62
1-chlorohexane	CCCCCCl	1-pentanol	-5.15	-9.66	-9.64
1-chlorooctane	CCCCCCCCCl	1-pentanol	-6.47	-11.90	-11.83
2-methyl-2-bromopropane	CC(C)(C)Br	1-pentanol	-3.58	-6.97	-7.15
2-methyl-2-chloropropane	CC(C)(C)Cl	1-pentanol	-3.25	-6.31	-6.46
2-methyl-2-iodopropane	CC(C)(C)I	1-pentanol	-4.22	-7.84	-7.56
2-methyl-2-bromobutane	CCC(C)(C)Br	1-pentanol	-4.17	-8.41	-8.14
1,2-dichloropropane	CC(Cl)CCl	1-pentanol	-4.80	-8.01	-8.68
1,3-dichloropropane	ClCCCCl	1-pentanol	-4.86	-8.91	-8.86
1,6-dichlorohexane	ClCCCCCCC1	1-pentanol	-7.10	-12.21	-12.26
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	1-pentanol	-8.15	-13.31	-13.63
trichloroethene	ClC=C(Cl)Cl	1-pentanol	-4.15	-8.13	-8.11
1,1-difluoroethane	CC(F)F	1-pentanol	-1.80	-3.99	-3.78
dimethyl carbonate	COC(=O)OC	1-pentanol	-3.82	-6.18	-6.88
diethyl carbonate	CCOC(=O)OCC	1-pentanol	-4.47	-8.66	-8.00
acetone	CC(C)=O	1-pentanol	-2.88	-6.79	-5.46
methyl ethyl ketone	CCC(C)=O	1-pentanol	-3.67	-6.73	-6.75
methyl isobutyl ketone	CC(C)CC(C)=O	1-pentanol	-5.01	-8.92	-9.13
2-heptanone	CCCCCC(C)=O	1-pentanol	-5.85	-9.90	-10.43
cyclohexanone	O=C1CCCCC1	1-pentanol	-6.12	-9.20	-10.89
butanal	CCCC=O	1-pentanol	-3.76	-6.29	-6.95
aniline	Nc1ccccc1	1-pentanol	-7.52	-12.65	-13.60
ethyl acetate	CCOC(C)=O	1-pentanol	-3.62	-6.33	-6.60
propyl acetate	CCCOC(C)=O	1-pentanol	-4.24	-6.94	-7.71
propyl formate	CCCOC=O	1-pentanol	-3.69	-7.55	-6.80
1-butylamine	CCCCN	1-pentanol	-5.15	-10.90	-11.24
1-heptylamine	CCCCCCCN	1-pentanol	-6.78	-14.32	-14.21
N-ethyl-N-butylamine	CCCCNCC	1-pentanol	-5.71	-12.36	-12.54
dipropylamine	CCCNCCC	1-pentanol	-5.54	-12.05	-12.30

dibutylamine	CCCCNCCCC	1-pentanol		-6.44	-14.51	-14.05
triethylamine	CCN(CC)CC	1-pentanol		-4.44	-10.44	-9.71
benzene	c1ccccc1	1-pentanol		-3.84	-7.53	-7.29
toluene	Cc1ccccc1	1-pentanol		-4.53	-8.57	-8.40
1,2,4-trimethylbenzene	Cc1ccc(C)c(C)c1	1-pentanol		-5.93	-10.91	-10.72
chlorobenzene	Clc1ccccc1	1-pentanol		-5.27	-9.28	-9.48
formamide	NC=O	1-pentanol		-6.77	-13.31	-13.60
tetramethylsilane	C[Si](C)(C)C	1-pentanol		-2.74	-5.54	-5.50
ethylene carbonate	O=C1OCCO1	1-pentanol		-4.95	-8.37	-9.10
diethyl malonate	CCOC(=O)CC(=O)OCC	1-pentanol		-7.37	-11.65	-12.87
$\beta$ -pinene	CC1(C)C2CCC(=C)C1C2	1-pentanol		-6.43	-10.57	-11.49
1,8-cineole	CC12CCC(CC1)C(C)C(O)2	1-pentanol		-6.51	-12.72	-11.23
1,3-diaminopropane	NCCCN	1-pentanol		-7.28	-15.58	-15.96
methylformamide	CNC=O	1-pentanol		-6.31	-12.16	-12.35
water	O	1-pentanol		-3.99	-9.88	-10.31
methane	C	1-butanol		0.55	-0.90	-0.78
isobutane	CC(C)C	1-butanol		-1.61	-4.27	-4.17
pentane	CCCCC	1-butanol		-2.49	-6.14	-5.60
hexane	CCCCCC	1-butanol		-3.22	-7.21	-6.77
heptane	CCCCCCC	1-butanol		-3.95	-8.32	-7.97
octane	CCCCCCCC	1-butanol		-4.64	-9.37	-9.17
nonane	CCCCCCCCC	1-butanol		-5.37	-10.17	-10.29
decane	CCCCCCCCC	1-butanol		-6.10	-11.56	-11.47
undecane	CCCCCCCCC	1-butanol		-6.71	-12.91	-12.53
dodecane	CCCCCCCCC	1-butanol		-7.43	-13.54	-13.73
tetradecane	CCCCCCCCC	1-butanol		-8.79	-16.24	-15.97
hexadecane	CCCCCCCCC	1-butanol		-10.15	-18.32	-18.12
3-ethylpentane	CCC(CC)CC	1-butanol		-3.66	-8.07	-7.51
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	1-butanol		-3.74	-8.05	-7.74
cyclooctane	C1CCCCCCC1	1-butanol		-5.27	-9.90	-9.86
propene	CC=C	1-butanol		-1.45	-3.37	-3.82
1-butene	CCC=C	1-butanol		-2.14	-4.42	-4.91
isobutene	CC(C)=C	1-butanol		-1.94	-4.40	-4.54
cis-2-butene	C/C=C/C	1-butanol		-2.09	-5.13	-4.77
trans-2-butene	C/C=C/C	1-butanol		-2.12	-4.74	-4.84
1,3-butadiene	C=CC=C	1-butanol		-2.44	-4.59	-5.29
methanol	CO	1-butanol		-3.60	-9.03	-8.54
ethanol	CCO	1-butanol		-4.18	-10.11	-9.60
propan-1-ol	CCCO	1-butanol		-4.95	-11.07	-10.91
butan-1-ol	CCCCO	1-butanol		-5.55	-12.45	-11.90
hexan-1-ol	CCCCCO	1-butanol		-6.92	-14.43	-14.23
2-butanol	CCC(C)O	1-butanol		-5.20	-11.97	-11.26
isobutanol	CC(C)CO	1-butanol		-5.53	-12.14	-11.88
dimethyl ether	COC	1-butanol		-1.98	-4.25	-4.27
diethyl ether	CCOCC	1-butanol		-3.08	-5.74	-6.02
methyl butyl ether	CCCCOC	1-butanol		-3.74	-7.26	-7.14
diisopropyl ether	CC(C)OC(C)C	1-butanol		-3.89	-7.56	-7.53
2-methyltetrahydrofuran	CC1CCCO1	1-butanol		-4.14	-7.54	-7.56
tetrahydropyran	C1CCOCC1	1-butanol		-4.23	-8.35	-7.70
1,4-dioxane	C1COCCO1	1-butanol		-4.61	-7.30	-8.43
18-crown-6	C1COCCOCCOCCOCCO1	1-butanol		-11.77	-21.14	-22.84
2,5,8,11,14-pentaoxopentadecane	CC(=O)CCC(=O)CCC(=O)CCC(=O)CCC(C)=O	1-butanol		-11.60	-16.43	-17.85
2-methyl-2-bromopropane	CC(C)(C)Br	1-butanol		-3.63	-7.04	-7.18
2-methyl-2-bromobutane	CCC(C)(C)Br	1-butanol		-4.21	-8.43	-8.15
dichloromethane	ClCCl	1-butanol		-3.12	-7.01	-6.25
chloroform	ClC(Cl)Cl	1-butanol		-4.02	-8.48	-7.85
tetrachloromethane	ClC(Cl)(Cl)Cl	1-butanol		-4.07	-7.80	-8.01
chloroethane	CCCl	1-butanol		-2.42	-5.60	-5.22
1-chlorobutane	CCCCCl	1-butanol		-3.94	-7.56	-7.65
2-chlorobutane	CCC(C)Cl	1-butanol		-3.78	-7.08	-7.38
1-chlorohexane	CCCCCCl	1-butanol		-5.19	-9.67	-9.67
2-methyl-2-chloropropane	CC(C)(C)Cl	1-butanol		-3.30	-6.42	-6.49
2-chloro-2-methylbutane	CCC(C)(C)Cl	1-butanol		-3.99	-7.73	-7.60
2-chloro-2-methylpentane	CCCC(C)(C)Cl	1-butanol		-4.61	-8.98	-8.60
trichloroethene	ClC=C(Cl)Cl	1-butanol		-4.31	-8.14	-8.34
helium	[He]	1-butanol		2.04	1.32	2.06
neon	[Ne]	1-butanol		1.87	1.56	1.71
argon	[Ar]	1-butanol		1.02	-0.57	0.19
krypton	[Kr]	1-butanol		0.42	-1.17	-0.67
hydrogen	[H][H]	1-butanol		1.53	-0.34	0.98
nitrogen	N#N	1-butanol		1.01	-0.39	0.16
oxygen	O=O	1-butanol		1.00	-0.29	-0.18
sulfur hexafluoride	F[S](F)(F)(F)(F)F	1-butanol		0.24	-1.86	-1.74
hydrogen sulfide	S	1-butanol		-1.55	-2.66	-2.76
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	1-butanol		-8.09	-13.32	-13.45
dimethyl carbonate	COC(=O)OC	1-butanol		-4.01	-7.12	-7.17
diethyl carbonate	CCOC(=O)OCC	1-butanol		-4.60	-8.52	-8.19
acetone	CC(C)=O	1-butanol		-3.11	-6.05	-5.85
methyl ethyl ketone	CCC(C)=O	1-butanol		-3.81	-6.44	-6.94
aniline	Nc1ccccc1	1-butanol		-7.54	-13.26	-13.53
methyl acetate	COC(C)=O	1-butanol		-3.50	-6.01	-6.33
ethyl acetate	CCOC(C)=O	1-butanol		-3.82	-6.93	-6.90

propyl acetate	CCCOC(C)=O	1-butanol	-4.38	-8.02	-7.91
butyl acetate	CCCCOC(C)=O	1-butanol	-4.97	-9.06	-8.91
pentyl acetate	CCCCCOC(C)=O	1-butanol	-5.62	-10.21	-10.02
methyl propanoate	CCC(=O)OC	1-butanol	-3.71	-7.02	-6.65
methyl heptanoate	CCCCCCC(=O)OC	1-butanol	-6.31	-10.90	-11.14
methyl nonanoate	CCCCCCCC(=O)OC	1-butanol	-7.63	-13.30	-13.41
ethyl propanoate	CCOC(=O)CC	1-butanol	-4.23	-7.33	-7.59
ethyl butanoate	CCCC(=O)OCC	1-butanol	-4.99	-8.78	-8.95
ethyl isobutyrate	CCOC(=O)C(C)C	1-butanol	-4.74	-8.00	-8.54
ethyl pentanoate	CCCCC(=O)OCC	1-butanol	-5.58	-9.95	-9.91
methyl benzoate	COC(=O)c1ccccc1	1-butanol	-7.22	-11.64	-12.00
ethyl benzoate	CCOC(=O)c1ccccc1	1-butanol	-7.91	-12.79	-13.24
propyl benzoate	CCCOC(=O)c1ccccc1	1-butanol	-8.55	-13.93	-14.40
butyl benzoate	CCCCOC(=O)c1ccccc1	1-butanol	-9.39	-14.96	-15.85
methyl lactate	COC(=O)C(C)O	1-butanol	-6.47	-11.68	-13.41
acetonitrile	CC#N	1-butanol	-4.04	-5.67	-6.53
butyronitrile	CCCC#N	1-butanol	-5.17	-7.65	-8.41
dimethyl sulfoxide	C[S](C)=O	1-butanol	-6.81	-11.17	-11.95
butylamine	CCCCN	1-butanol	-5.17	-10.95	-11.19
1-heptylamine	CCCCCCCN	1-butanol	-6.79	-14.27	-14.14
dibutylamine	CCCCNCCCC	1-butanol	-6.42	-14.53	-13.94
triethylamine	CCN(CC)CC	1-butanol	-4.42	-10.31	-9.57
tributylamine	CCCCN(CCCC)CCCC	1-butanol	-7.65	-15.75	-15.38
1,3-diaminopropane	NCCCN	1-butanol	-7.28	-15.61	-15.95
pyridine	c1ccncc1	1-butanol	-5.37	-9.66	-9.02
2-methylpyridine	Cc1cccn1	1-butanol	-6.19	-11.04	-10.56
3-methylpyridine	Cc1ccncc1	1-butanol	-6.21	-11.02	-10.51
4-ethylpyridine	CCc1ccncc1	1-butanol	-6.95	-12.17	-11.75
3-chloropyridine	Clc1ccncc1	1-butanol	-6.92	-10.83	-11.31
benzene	c1ccccc1	1-butanol	-3.89	-7.49	-7.32
toluene	Cc1ccccc1	1-butanol	-4.66	-8.57	-8.58
chlorobenzene	Clc1ccccc1	1-butanol	-5.25	-9.47	-9.37
1,2-dichlorobenzene	Clc1ccccc1Cl	1-butanol	-6.46	-11.60	-11.41
nitrobenzene	[O-][N+](=O)c1ccccc1	1-butanol	-7.02	-11.35	-11.89
1,1-difluoroethane	CC(F)F	1-butanol	-1.90	-4.12	-3.87
fluoromethane	CF	1-butanol	-0.51	-2.64	-2.01
difluoromethane	FCF	1-butanol	-0.98	-1.80	-2.51
benzamide	NC(=O)c1ccccc1	1-butanol	-10.88	-19.39	-19.20
benzoic acid	OC(=O)c1ccccc1	1-butanol	-9.47	-17.84	-17.76
tetramethylsilane	C[Si](C)(C)C	1-butanol	-2.80	-5.57	-5.51
benzaldehyde	O=Cc1ccccc1	1-butanol	-6.44	-10.38	-10.79
acetophenone	CC(=O)c1ccccc1	1-butanol	-7.26	-11.30	-12.16
N-methylpyrrole	Cn1ccccc1	1-butanol	-5.21	-8.51	-9.86
β-pinene	CC1(C)C2CCC(=C)C1C2	1-butanol	-6.33	-10.68	-11.21
1,8-cineole	CC12CCC(CC1)C(C)C2O	1-butanol	-6.54	-12.74	-11.23
linalool	CC(C)=CCCC(C)(O)C=C	1-butanol	-8.25	-15.76	-15.97
formamide	NC=O	1-butanol	-6.93	-13.38	-13.84
methylformamide	CNC=O	1-butanol	-6.49	-12.24	-12.63
dimethylformamide	CN(C)C=O	1-butanol	-5.55	-10.28	-10.69
water	O	1-butanol	-4.05	-10.10	-10.30
tetramethylstannane	C[Sn](C)(C)C	1-butanol	-3.84	-7.30	-7.16
methane	C	1-hexanol	0.59	-0.50	-0.73
ethane	CC	1-hexanol	-0.27	-2.10	-2.15
pentane	CCCCC	1-hexanol	-2.48	-6.19	-5.68
hexane	CCCCCC	1-hexanol	-3.27	-7.33	-6.98
nonane	CCCCCCCCC	1-hexanol	-5.47	-10.73	-10.63
dodecane	CCCCCCCCCCCC	1-hexanol	-7.54	-14.05	-14.08
hexadecane	CCCCCCCCCCCCCCCC	1-hexanol	-10.30	-18.59	-18.55
3-methylpentane	CCC(C)CC	1-hexanol	-3.09	-7.00	-6.74
2,2-dimethylbutane	CCC(C)(C)C	1-hexanol	-2.41	-6.37	-5.54
2,3-dimethylbutane	CC(C)(C)C	1-hexanol	-2.91	-6.73	-6.44
3-ethylpentane	CCC(C)CC	1-hexanol	-3.76	-8.17	-7.85
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	1-hexanol	-3.74	-8.11	-7.84
cyclohexane	C1CCCCC1	1-hexanol	-3.90	-7.54	-7.74
methylcyclohexane	CC1CCCCC1	1-hexanol	-4.48	-8.04	-8.72
cyclooctane	C1CCCCCCC1	1-hexanol	-5.35	-9.97	-10.17
bicyclohexyl	C1CCC(CC1)C2CCCCC2	1-hexanol	-7.94	-13.48	-13.67
hexan-1-ol	CCCCCCO	1-hexanol	-6.80	-14.72	-14.12
octan-1-ol	CCCCCCCCO	1-hexanol	-8.36	-16.94	-16.63
decan-1-ol	CCCCCCCCCO	1-hexanol	-9.61	-19.37	-18.67
dibutyl ether	CCCCOCCCC	1-hexanol	-5.76	-10.23	-10.70
diisopropyl ether	CC(C)OC(C)C	1-hexanol	-3.68	-7.45	-7.23
1,2-dimethoxyethane	COCCOC	1-hexanol	-4.47	-7.64	-8.42
2-methyl-2-bromopropane	CC(C)(C)Br	1-hexanol	-3.54	-6.92	-7.13
chloroform	ClC(Cl)Cl	1-hexanol	-3.79	-8.27	-7.52
tetrachloromethane	ClC(Cl)(Cl)Cl	1-hexanol	-3.87	-7.72	-7.75
1-chlorobutane	CCCCCl	1-hexanol	-3.75	-7.48	-7.41
1-chlorohexane	CCCCCCC1	1-hexanol	-5.12	-9.65	-9.65
2-methyl-2-chloropropane	CC(C)(C)Cl	1-hexanol	-3.20	-6.28	-6.44
trichloroethene	ClC=C(Cl)Cl	1-hexanol	-4.07	-8.15	-8.02
1,5-dichloropentane	ClCCCCCl	1-hexanol	-6.41	-10.94	-11.22
1,6-dichlorohexane	ClCCCCCl	1-hexanol	-7.03	-12.17	-12.19
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	1-hexanol	-6.43	-11.18	-11.53

2-methyl-2-iodopropane	CC(C)(C)I	1-hexanol	-4.26	-7.83	-7.71
xenon	[Xe]	1-hexanol	-0.47	-2.36	-2.37
diethyl carbonate	CCOC(=O)OCC	1-hexanol	-4.42	-8.67	-8.00
methyl ethyl ketone	CCC(C)=O	1-hexanol	-3.53	-6.70	-6.56
2-octanone	CCCCCCC(=O)	1-hexanol	-6.55	-11.09	-11.65
methyl isobutyl ketone	CC(C)CC(C)=O	1-hexanol	-4.92	-9.29	-9.02
ethyl acetate	CCOC(C)=O	1-hexanol	-3.39	-6.81	-6.25
butyl acetate	CCCCOC(C)=O	1-hexanol	-4.72	-8.86	-8.57
methyl pentanoate	CCCCC(=O)OC	1-hexanol	-4.86	-8.90	-8.76
methyl heptanoate	CCCCCCC(=O)OC	1-hexanol	-6.21	-11.19	-11.12
methyl nonanoate	CCCCCCCCC(=O)OC	1-hexanol	-7.55	-13.33	-13.39
methyl undecanoate	CCCCCCCCCCC(=O)OC	1-hexanol	-9.00	-15.54	-15.86
methyl tridecanoate	CCCCCCCCCCCCC(=O)OC	1-hexanol	-9.91	-18.27	-17.97
methyl pentadecanoate	CCCCCCCCCCCCCCC(=O)OC	1-hexanol	-11.77	-20.76	-20.30
ethyl propanoate	CCOC(=O)CC	1-hexanol	-4.14	-8.91	-7.61
acetonitrile	CC#N	1-hexanol	-3.64	-5.69	-5.92
butyronitrile	CCCC#N	1-hexanol	-4.83	-7.36	-7.91
butylamine	CCCCN	1-hexanol	-5.13	-10.64	-11.28
dibutylamine	CCCCNCCCC	1-hexanol	-6.46	-14.44	-14.14
triethylamine	CCN(CC)CC	1-hexanol	-4.48	-10.37	-9.83
pyridine	c1ccncc1	1-hexanol	-5.36	-9.63	-9.23
2-methylpyridine	Cc1cccc1	1-hexanol	-6.07	-11.02	-10.50
3-methylpyridine	Cc1ccncc1	1-hexanol	-6.17	-10.97	-10.65
benzene	c1ccccc1	1-hexanol	-3.83	-7.51	-7.34
benzonitrile	N#Cc1ccccc1	1-hexanol	-7.24	-10.15	-11.24
anisole	COc1ccccc1	1-hexanol	-5.44	-9.97	-9.46
nitrobenzene	[O-][N+](=O)c1ccccc1	1-hexanol	-6.66	-11.50	-11.35
tetramethylsilane	C[Si](C)(C)C	1-hexanol	-2.70	-5.57	-5.51
ethylene carbonate	O=C1OCCO1	1-hexanol	-4.85	-8.51	-8.99
hexanoic acid	CCCCC(O)=O	1-hexanol	-7.69	-16.61	-15.75
octanoic acid	CCCCCCC(O)=O	1-hexanol	-9.58	-18.89	-18.92
2-methylphenol	Cc1ccccc1O	1-hexanol	-8.16	-15.43	-15.64
formamide	NC=O	1-hexanol	-6.58	-13.29	-13.31
methylformamide	CNC=O	1-hexanol	-6.12	-12.14	-12.03
dimethylformamide	CN(C)C=O	1-hexanol	-5.23	-9.73	-10.18
naphthalene	c1ccc2ccccc2c1	1-hexanol	-7.28	-12.61	-12.72
biphenyl	c1ccc(cc1)c2ccccc2	1-hexanol	-8.81	-14.86	-14.91
1-nitronaphthalene	[O-][N+](=O)c1ccc2ccccc12	1-hexanol	-10.04	-17.09	-16.67
water	O	1-hexanol	-3.94	-9.79	-10.30
propane	CCC	isopropanol	-1.26	-3.38	-3.39
isobutane	CC(C)C	isopropanol	-1.78	-4.28	-4.21
hexane	CCCCCC	isopropanol	-3.32	-6.97	-6.67
heptane	CCCCCCC	isopropanol	-4.03	-7.80	-7.82
nonane	CCCCCCCCC	isopropanol	-5.38	-10.22	-10.02
dodecane	CCCCCCCCCCCC	isopropanol	-7.43	-13.36	-13.44
hexadecane	CCCCCCCCCCCCCCCC	isopropanol	-9.95	-17.66	-17.41
3-ethylpentane	CCC(CC)CC	isopropanol	-3.77	-7.81	-7.43
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	isopropanol	-3.90	-7.77	-7.78
cyclohexane	C1CCCCC1	isopropanol	-3.75	-7.37	-6.95
cyclooctane	C1CCCCCCC1	isopropanol	-5.12	-9.61	-9.20
bicyclohexyl	C1CCC(CC1)C2CCCCC2	isopropanol	-7.52	-12.99	-12.32
1-propene	CC=C	isopropanol	-1.63	-4.20	-3.88
1-butene	CCC=C	isopropanol	-2.32	-4.98	-4.98
cis-2-butene	C/C=C/C	isopropanol	-2.27	-4.90	-4.84
1-heptene	CCCCC=C	isopropanol	-4.25	-7.90	-8.05
isobutene	CC(C)=C	isopropanol	-2.12	-4.94	-4.61
1,3-butadiene	C=CC=C	isopropanol	-2.63	-4.91	-5.36
acetylene	C#C	isopropanol	-1.45	-4.02	-3.70
methanol	CO	isopropanol	-3.74	-9.04	-8.49
ethanol	CCO	isopropanol	-4.31	-10.16	-9.54
propan-1-ol	CCCO	isopropanol	-5.07	-11.36	-10.83
butan-1-ol	CCCCO	isopropanol	-5.66	-12.52	-11.79
hexan-1-ol	CCCCCO	isopropanol	-6.98	-14.62	-13.98
decan-1-ol	CCCCCCCCCO	isopropanol	-9.61	-18.98	-18.14
isopropanol	CC(C)O	isopropanol	-4.75	-10.84	-10.34
3-methyl-1-butanol	CC(C)CCO	isopropanol	-6.31	-13.38	-12.82
2-methyl-2-butanol	CCC(C)(C)O	isopropanol	-5.07	-12.36	-10.79
benzene	c1ccccc1	isopropanol	-4.10	-7.54	-7.46
toluene	Cc1ccccc1	isopropanol	-4.76	-8.19	-8.50
1,2-dimethylbenzene	Cc1ccccc1C	isopropanol	-5.37	-9.38	-9.50
1,3-dimethylbenzene	Cc1cccc(C)c1	isopropanol	-5.34	-9.59	-9.42
1,4-dimethylbenzene	Cc1ccc(C)cc1	isopropanol	-5.34	-9.24	-9.41
chloroform	ClC(Cl)Cl	isopropanol	-4.23	-8.46	-7.98
tetrachloromethane	ClC(Cl)(Cl)Cl	isopropanol	-4.25	-7.49	-8.08
chloroethane	CCCl	isopropanol	-2.53	-5.29	-5.16
2-chloro-2-methylpropane	CC(C)(C)Cl	isopropanol	-3.29	-6.07	-6.18
2-chloro-2-methylbutane	CCC(C)(C)Cl	isopropanol	-3.98	-7.36	-7.29
trichloroethene	ClC=C(Cl)Cl	isopropanol	-4.51	-8.28	-8.47
2-bromopropane	CC(C)Br	isopropanol	-3.40	-6.48	-6.56
2-methyl-2-bromopropane	CC(C)(C)Br	isopropanol	-3.59	-6.62	-6.81
1,1-difluoroethane	CC(F)F	isopropanol	-2.13	-4.09	-4.03
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	isopropanol	-7.89	-12.82	-12.71
acetone	CC(C)=O	isopropanol	-3.38	-5.73	-6.10

methyl ethyl ketone	CCC(C)=O	isopropanol	-4.03	-6.95	-7.10
dimethyl ether	COC	isopropanol	-2.14	-4.21	-4.29
dibutyl ether	CCCCOCCCC	isopropanol	-5.84	-9.80	-10.44
tetrahydrofuran	C1CCOC1	isopropanol	-3.63	-5.93	-6.38
1,4-dioxane	C1COCCO1	isopropanol	-4.64	-7.04	-8.10
15-crown-5	C1COCCOCCOCCOCCO1	isopropanol	-10.42	-16.52	-19.88
18-crown-6	C1COCCOCCOCCOCCOCCO1	isopropanol	-11.73	-20.67	-22.41
aniline	Nc1ccccc1	isopropanol	-7.47	-12.04	-13.06
krypton	[Kr]	isopropanol	0.30	-1.57	-0.62
xenon	[Xe]	isopropanol	-0.71	-2.19	-2.37
nitrogen	N#N	isopropanol	0.98	0.71	0.41
carbon monoxide	C=O	isopropanol	0.71	-0.52	-0.26
carbon dioxide	O=C=O	isopropanol	-0.73	-1.97	-2.86
oxygen	O=O	isopropanol	1.11	0.07	0.30
propyl formate	CCCOC=O	isopropanol	-3.94	-7.18	-6.85
methyl acetate	COC(C)=O	isopropanol	-3.75	-5.69	-6.51
ethyl acetate	CCOC(C)=O	isopropanol	-4.08	-6.96	-7.09
propyl acetate	CCCOC(C)=O	isopropanol	-4.60	-7.54	-8.03
butyl acetate	CCCCOC(C)=O	isopropanol	-5.15	-9.05	-8.97
isobutyl acetate	CC(C)COC(C)=O	isopropanol	-5.11	-7.93	-9.00
pentyl acetate	CCCCCOC(C)=O	isopropanol	-5.83	-9.89	-10.14
isopentyl acetate	CC(C)CCOC(C)=O	isopropanol	-5.77	-9.48	-10.15
propyl propionate	CCCOC(=O)CC	isopropanol	-5.00	-8.15	-8.70
methyl butanoate	CCCC(=O)OC	isopropanol	-4.56	-7.76	-7.87
propyl butanoate	CCCOC(=O)CCC	isopropanol	-5.89	-8.93	-10.28
acetonitrile	CC#N	isopropanol	-4.28	-5.72	-6.73
1-butylamine	CCCCN	isopropanol	-5.27	-10.30	-11.07
isobutylamine	CC(C)CN	isopropanol	-4.93	-10.40	-10.73
tert-butylamine	CC(C)(C)N	isopropanol	-3.99	-9.32	-9.58
1-heptylamine	CCCCCCN	isopropanol	-6.76	-13.70	-13.72
triethylamine	CCN(CC)CC	isopropanol	-4.38	-9.65	-9.13
tripropylamine	CCCN(CCC)CCC	isopropanol	-5.93	-11.06	-12.02
chlorobenzene	Clc1ccccc1	isopropanol	-5.22	-9.03	-9.02
nitromethane	C[N+](=O)[O-]	isopropanol	-4.29	-6.61	-7.98
4-methylpyridine	Cc1ccncc1	isopropanol	-6.32	-10.66	-10.41
1,3-dimethoxybenzene	COc1ccc(OC)c1	isopropanol	-7.67	-13.28	-12.76
tetramethylsilane	C[Si](C)(C)C	isopropanol	-2.90	-5.31	-5.34
adipic acid	OC(=O)CCCC(O)=O	isopropanol	-12.74	-25.24	-25.63
ethylene carbonate	O=C1OCCO1	isopropanol	-5.24	-7.36	-9.24
acenaphthene	C1Cc2ccc3cccc1c23	isopropanol	-8.83	-13.54	-14.53
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	isopropanol	-9.75	-17.62	-17.04
quinoline	c1ccc2ncccc2c1	isopropanol	-9.26	-13.62	-15.01
benzamide	NC(=O)c1ccccc1	isopropanol	-11.00	-19.04	-19.36
benzoic acid	OC(=O)c1ccccc1	isopropanol	-9.54	-17.45	-17.58
1,2-epoxybutane	CCC1CO1	isopropanol	-3.65	-6.91	-6.38
dichlorodifluoromethane	FC(F)(Cl)Cl	isopropanol	-1.80	-3.90	-4.83
1,1,2,2-tetrafluoroethane	FC(F)C(F)F	isopropanol	-2.51	-3.47	-4.26
pentafluoroethane	FC(F)C(F)(F)F	isopropanol	-1.88	-3.61	-3.74
diethyl malonate	CCOC(=O)CC(=O)OCC	isopropanol	-7.79	-11.14	-13.32
sebacic acid	OC(=O)CCCCCCCC(O)=O	isopropanol	-14.46	-28.21	-29.20
R-fenchone	C[C@H]12CCC(C(C)(C)C2=O)C1	isopropanol	-7.84	-10.82	-12.96
N-methylimidazole	Cn1ccnc1	isopropanol	-7.00	-13.16	-11.69
methane	C	tetrahydrofuran	0.04	-0.72	-0.90
ethane	CC	tetrahydrofuran	-0.84	-3.28	-2.28
propane	CCC	tetrahydrofuran	-1.60	-3.99	-3.51
hexane	CCCCCC	tetrahydrofuran	-3.76	-6.79	-6.92
heptane	CCCCCCC	tetrahydrofuran	-4.44	-7.98	-7.98
octane	CCCCCCCC	tetrahydrofuran	-5.04	-8.97	-8.85
nonane	CCCCCCCCC	tetrahydrofuran	-5.76	-10.07	-10.01
dodecane	CCCCCCCCCCCC	tetrahydrofuran	-7.70	-13.51	-13.06
tetradecane	CCCCCCCCCCCCC	tetrahydrofuran	-8.96	-15.38	-15.06
3-methylpentane	CCC(C)CC	tetrahydrofuran	-3.62	-6.52	-6.71
2,2-dimethylbutane	CCC(C)(C)C	tetrahydrofuran	-3.01	-5.93	-5.65
2,3-dimethylbutane	CC(C)(C)C	tetrahydrofuran	-3.48	-6.26	-6.48
cyclohexane	C1CCCCC1	tetrahydrofuran	-3.97	-7.02	-6.78
methylcyclohexane	CC1CCCCC1	tetrahydrofuran	-4.45	-7.86	-7.50
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	tetrahydrofuran	-4.17	-7.86	-7.46
1-hexene	CCCC=C	tetrahydrofuran	-4.16	-6.97	-7.65
trichloromethane	ClC(Cl)Cl	tetrahydrofuran	-4.80	-9.47	-8.74
tetrachloromethane	ClC(Cl)(Cl)Cl	tetrahydrofuran	-4.83	-8.54	-8.63
chlorocyclohexane	C1CCCCC1	tetrahydrofuran	-5.81	-10.30	-9.84
trichloroethene	ClC=C(Cl)Cl	tetrahydrofuran	-5.04	-9.49	-9.08
tetrachloroethene	ClC(Cl)=C(Cl)Cl	tetrahydrofuran	-5.25	-9.72	-9.37
dipropyl ether	CCOCCC	tetrahydrofuran	-4.71	-8.27	-8.08
diisopropyl ether	CC(C)OC(C)C	tetrahydrofuran	-4.33	-7.50	-7.56
dibutyl ether	CCCCOCCCC	tetrahydrofuran	-5.90	-10.55	-9.84
methyl tert-butyl ether	COC(C)(C)C	tetrahydrofuran	-3.67	-7.16	-6.54
tetrahydrofuran	C1CCOC1	tetrahydrofuran	-3.93	-7.65	-6.65
ethyl benzoate	CCOC(=O)c1ccccc1	tetrahydrofuran	-8.79	-14.75	-14.72
butyl benzoate	CCCCOC(=O)c1ccccc1	tetrahydrofuran	-10.00	-16.78	-16.60
methanol	CO	tetrahydrofuran	-3.91	-8.10	-8.49
ethanol	CCO	tetrahydrofuran	-4.57	-9.08	-9.60
isopropanol	CC(C)O	tetrahydrofuran	-4.95	-9.14	-10.18

1-heptanol	CCCCCCCO	tetrahydrofuran	-7.67	-14.76	-14.27
1-octanol	CCCCCCCCO	tetrahydrofuran	-8.26	-15.68	-15.09
1-decanol	CCCCCCCCCO	tetrahydrofuran	-9.21	-18.00	-16.60
2-methoxyethanol	COCCO	tetrahydrofuran	-5.76	-10.23	-11.49
acetonitrile	CC#N	tetrahydrofuran	-4.61	-8.05	-7.45
benzene	c1ccccc1	tetrahydrofuran	-4.78	-8.42	-8.48
1,4-dimethylbenzene	Cc1ccc(C)cc1	tetrahydrofuran	-6.03	-10.33	-10.50
anisole	COc1ccccc1	tetrahydrofuran	-6.52	-11.69	-11.12
chlorobenzene	Clc1ccccc1	tetrahydrofuran	-5.95	-10.46	-10.26
fluorobenzene	Fc1ccccc1	tetrahydrofuran	-4.90	-8.99	-8.66
benzyl chloride	ClCc1ccccc1	tetrahydrofuran	-6.70	-12.61	-11.28
pyrrole	[nH]1ccccc1	tetrahydrofuran	-6.40	-12.73	-11.43
N-methylpyrrole	Cn1ccccc1	tetrahydrofuran	-5.43	-9.93	-9.31
aniline	Nc1ccccc1	tetrahydrofuran	-8.14	-15.02	-14.46
helium	[He]	tetrahydrofuran	2.13	1.94	2.25
neon	[Ne]	tetrahydrofuran	1.96	1.68	1.90
argon	[Ar]	tetrahydrofuran	0.69	-0.01	0.05
hydrogen	[H][H]	tetrahydrofuran	1.33	1.07	0.88
deuterium	[H][H]	tetrahydrofuran	1.33	1.44	0.88
nitrogen	N#N	tetrahydrofuran	0.85	0.32	0.64
carbon dioxide	O=C=O	tetrahydrofuran	-0.88	-4.07	-2.58
sulfur hexafluoride	F[S](F)(F)(F)(F)F	tetrahydrofuran	0.46	1.15	-0.51
pyridine	c1ccncc1	tetrahydrofuran	-5.94	-9.46	-9.65
3-methylpyridine	Cc1ccncc1	tetrahydrofuran	-6.75	-10.52	-11.05
hexafluorobenzene	Fc1c(F)c(F)c(F)c(F)c1F	tetrahydrofuran	-3.62	-8.48	-7.94
sulfur dioxide	O=[S]=O	tetrahydrofuran	-3.50	-9.39	-7.67
15-crown-5	C1COCCOCCOCCOCCO1	tetrahydrofuran	-10.59	-18.86	-19.32
phenol	Oc1ccccc1	tetrahydrofuran	-8.39	-16.97	-15.79
4-fluorophenol	Oc1ccc(F)cc1	tetrahydrofuran	-9.04	-17.83	-17.37
1-chloronaphthalene	Clc1cccc2ccccc12	tetrahydrofuran	-9.11	-16.34	-15.19
1-methylnaphthalene	Cc1cccc2ccccc12	tetrahydrofuran	-8.68	-14.40	-14.65
diethyl carbonate	CCOC(=O)OCC	tetrahydrofuran	-5.39	-10.11	-9.09
propylamine	CCCN	tetrahydrofuran	-4.56	-7.23	-8.89
isopropylamine	CC(C)N	tetrahydrofuran	-3.95	-6.59	-8.09
isobutylamine	CC(C)CN	tetrahydrofuran	-4.88	-7.91	-9.69
tert-butylamine	CC(C)(C)N	tetrahydrofuran	-4.08	-6.98	-8.79
diethylamine	CCNCC	tetrahydrofuran	-4.48	-7.95	-8.92
dipropylamine	CCCNCCC	tetrahydrofuran	-5.49	-9.59	-10.75
dibutylamine	CCCNCCCC	tetrahydrofuran	-6.44	-11.44	-12.55
diisopropylamine	CC(C)NC(C)C	tetrahydrofuran	-4.66	-8.00	-9.68
triethylamine	CCN(CC)CC	tetrahydrofuran	-4.50	-7.96	-8.40
tripropylamine	CCCN(CCC)CCC	tetrahydrofuran	-6.11	-10.11	-11.35
tributylamine	CCCN(CCCC)CCCC	tetrahydrofuran	-7.85	-14.01	-14.32
hexanoic acid	CCCCCC(O)=O	tetrahydrofuran	-8.29	-17.16	-15.89
octanoic acid	CCCCCCCC(O)=O	tetrahydrofuran	-9.84	-19.81	-18.33
4-fluoroanisole	COc1ccc(F)cc1	tetrahydrofuran	-7.32	-12.39	-12.99
formamide	NC=O	tetrahydrofuran	-7.26	-14.29	-14.39
dimethylformamide	CN(C)C=O	tetrahydrofuran	-6.27	-10.83	-11.51
N,N-dimethylacetamide	CN(C)C(C)=O	tetrahydrofuran	-6.76	-11.93	-12.32
2-pyrrolidone	O=C1CCCN1	tetrahydrofuran	-8.91	-15.30	-16.27
3-methoxyphenol	COc1cccc(O)c1	tetrahydrofuran	-9.97	-19.69	-18.37
3-chlorophenol	Oc1cccc(Cl)c1	tetrahydrofuran	-9.52	-19.19	-17.50
3-nitrophenol	Oc1cccc(c1)[N+](=O)[O-]	tetrahydrofuran	-10.99	-22.28	-20.33
4-nitrophenol	Oc1ccc(cc1)[N+](=O)[O-]	tetrahydrofuran	-11.06	-22.47	-20.43
1,3-dihydroxyphenol	OC1=CC=CC(O)C1	tetrahydrofuran	-11.30	-24.88	-22.81
1,4-dihydroxyphenol	OC1=CCC(O)C=C1	tetrahydrofuran	-11.46	-24.76	-22.94
1-naphthol	Oc1cccc2ccccc12	tetrahydrofuran	-11.37	-22.47	-20.35
2,6-di-tert-butylphenol	CC(C)(C)c1ccc(c1O)C(C)(C)C	tetrahydrofuran	-10.42	-19.50	-18.78
anthracene	c1ccc2cc3ccccc3cc2c1	tetrahydrofuran	-11.18	-19.60	-18.50
azulene	c1ccc2ccccc2cc1	tetrahydrofuran	-7.98	-14.10	-13.50
chrysene	c1ccc2c(c1)ccc3c4ccccc4ccc23	tetrahydrofuran	-14.39	-24.74	-23.55
benz[a]anthracene	c1ccc2cc3c(ccc4ccccc34)cc2c1	tetrahydrofuran	-14.38	-25.10	-23.51
pyrazole	[nH]1cccn1	tetrahydrofuran	-7.19	-14.36	-12.87
1-methylpyrazole	Cn1cccn1	tetrahydrofuran	-5.89	-10.74	-9.82
3-methyl-1h-pyrazole	Cc1cc[nH]n1	tetrahydrofuran	-8.08	-14.96	-14.50
1,3,5-trimethylpyrazole	Cn1nc(C)cc1C	tetrahydrofuran	-6.78	-13.00	-11.35
water	O	tetrahydrofuran	-4.07	-9.50	-9.48
indole	[nH]1ccc2ccccc12	tetrahydrofuran	-9.51	-16.01	-16.30
phenoxazine	N1c2ccccc2Oc3ccccc13	tetrahydrofuran	-14.20		-23.97
phenthiazine	N1c2ccccc2Sc3ccccc13	tetrahydrofuran	-15.11		-24.92
1,2,4-triazole	[nH]1cnen1	tetrahydrofuran	-7.52		-13.31
phthalimide	O=C1NC(=O)c2ccccc12	tetrahydrofuran	-13.43		-23.65
γ-butyrolactam	O=C1CCCN1	tetrahydrofuran	-8.91	-16.40	-16.26
N-methylbutyrolactam	CN1CCCC1=O	tetrahydrofuran	-7.67	-13.10	-13.40
N-methylvalerolactam	CN1CCCCC1=O	tetrahydrofuran	-8.10	-13.93	-14.04
ε-caprolactam	O=C1CCCCCN1	tetrahydrofuran	-9.37	-16.42	-16.73
N-methylcaprolactam	CN1CCCCC1=O	tetrahydrofuran	-8.45	-14.72	-14.54
tetramethylstannane	C[Sn](C)(C)C	tetrahydrofuran	-4.09	-7.20	-6.63
N-methylimidazole	Cn1ccnc1	tetrahydrofuran	-7.37	-12.63	-12.32
helium	[He]	dichloromethane	1.94	2.68	1.85
argon	[Ar]	dichloromethane	0.54	0.92	-0.21
hydrogen	[H][H]	dichloromethane	1.48	2.12	1.08
oxygen	O=O	dichloromethane	0.85	0.85	0.25

carbon dioxide	O=C=O	dichloromethane	-1.04	-2.62	-3.08
pentane	CCCCC	dichloromethane	-2.83	-4.79	-5.44
hexane	CCCCCC	dichloromethane	-3.53	-5.86	-6.55
2-methylpentane	CCCC(C)C	dichloromethane	-3.33	-5.48	-6.23
heptane	CCCCCCC	dichloromethane	-4.22	-6.83	-7.67
octane	CCCCCCCC	dichloromethane	-4.85	-7.81	-8.73
nonane	CCCCCCCCC	dichloromethane	-5.57	-8.85	-9.85
decane	CCCCCCCCC	dichloromethane	-6.28	-9.69	-10.97
dodecane	CCCCCCCCCCC	dichloromethane	-7.53	-11.74	-13.07
hexadecane	CCCCCCCCCCCCCCC	dichloromethane	-9.99	-15.54	-16.92
1-octene	CCCCCCC=C	dichloromethane	-5.11	-8.40	-8.98
isoprene	CC(=C)C=C	dichloromethane	-3.14	-6.15	-5.80
cyclopentadiene	C1C=CC=C1	dichloromethane	-3.74	-6.69	-6.75
1,3-cyclopentadiene	C1C=CC=C1	dichloromethane	-3.75	-7.64	-6.75
dichloromethane	ClCCl	dichloromethane	-3.38	-6.88	-6.13
trichloromethane	ClC(Cl)Cl	dichloromethane	-4.13	-7.42	-7.34
tetrachloromethane	ClC(Cl)(Cl)Cl	dichloromethane	-4.32	-7.19	-7.74
1-chloropropane	CCCCl	dichloromethane	-3.83	-6.74	-7.12
1,2-dichloroethane	ClCCCl	dichloromethane	-4.59	-8.48	-8.04
1,6-dichlorohexane	ClCCCCCl	dichloromethane	-7.86	-13.73	-13.20
diethyl ether	CCOCC	dichloromethane	-4.07	-7.09	-7.50
dibutyl ether	CCCCOCCCC	dichloromethane	-6.62	-10.12	-11.72
furan	c1cccl	dichloromethane	-4.54	-6.73	-8.10
tetrahydropyran	C1CCOCC1	dichloromethane	-5.41	-9.48	-9.57
1,4-dioxane	C1COCCO1	dichloromethane	-5.57	-10.46	-9.81
propanone	CC(C)=O	dichloromethane	-4.31	-8.31	-7.83
pentane-2-one	CCCC(C)=O	dichloromethane	-5.63	-9.83	-9.94
heptan-2-one	CCCCCC(C)=O	dichloromethane	-6.86	-11.73	-11.94
octan-2-one	CC(CCCCCC)=O	dichloromethane	-7.61	-12.66	-13.11
cyclohexanone	O=C1CCCCC1	dichloromethane	-6.82	-12.03	-11.63
butyl formate	CCCCOC=O	dichloromethane	-5.96	-10.32	-10.53
methyl acetate	COC(C)=O	dichloromethane	-4.95	-8.37	-8.80
ethyl acetate	CCOC(C)=O	dichloromethane	-5.36	-8.99	-9.51
butyl acetate	CCCCOC(C)=O	dichloromethane	-6.47	-10.56	-11.41
methyl propionate	CCC(=O)OC	dichloromethane	-5.22	-9.20	-9.24
propionitrile	CCC#N	dichloromethane	-5.78	-9.52	-9.40
diethylamine	CCNCC	dichloromethane	-4.65	-7.86	-9.49
triethylamine	CCN(CC)CC	dichloromethane	-5.01	-8.60	-9.94
nitromethane	C[N+](=O)[O-]	dichloromethane	-5.00	-8.95	-9.21
1-nitropropane	CCC[N+](=O)[O-]	dichloromethane	-6.27	-10.83	-11.14
propan-1-ol	CCCO	dichloromethane	-4.55	-8.15	-8.97
butan-1-ol	CCCCO	dichloromethane	-5.11	-9.01	-9.88
2-butanol	CCC(C)O	dichloromethane	-4.91	-8.31	-9.56
pentan-1-ol	CCCCCO	dichloromethane	-5.85	-10.08	-11.11
hexan-1-ol	CCCCCCO	dichloromethane	-6.43	-10.98	-12.07
octan-1-ol	CCCCCCCCO	dichloromethane	-7.80	-12.78	-14.17
decan-1-ol	CCCCCCCCCO	dichloromethane	-9.04	-14.99	-16.20
formamide	NC=O	dichloromethane	-6.74	-11.79	-12.95
dimethylformamide	CN(C)C=O	dichloromethane	-6.40	-12.70	-11.92
N,N-dimethylacetamide	CN(C)C(C)=O	dichloromethane	-7.00	-13.69	-13.15
diethyl carbonate	CCOC(=O)OCC	dichloromethane	-6.17	-11.35	-10.85
benzene	c1ccccc1	dichloromethane	-4.58	-7.96	-8.11
toluene	Cc1ccccc1	dichloromethane	-5.20	-9.20	-9.08
ethylbenzene	CCc1ccccc1	dichloromethane	-5.87	-9.84	-10.08
o-xylene	Cc1ccccc1C	dichloromethane	-5.81	-10.09	-10.05
p-xylene	Cc1ccc(C)cc1	dichloromethane	-5.84	-10.23	-10.08
naphthalene	c1ccc2ccccc2c1	dichloromethane	-7.94	-12.91	-13.39
biphenyl	c1ccc(cc1)c2ccccc2	dichloromethane	-9.55	-15.06	-15.78
anthracene	c1ccc2cc3ccccc3cc2c1	dichloromethane	-11.31	-18.59	-18.70
1,3-diphenylbenzene	c1ccc(cc1)c2ccccc2c3ccccc3	dichloromethane	-13.81	-22.85	-22.02
1-chloronaphthalene	Clc1ccc2ccccc2c1	dichloromethane	-9.19	-15.19	-15.23
aniline	Nc1ccccc1	dichloromethane	-7.36	-12.01	-12.35
pyrrole	[nH]1ccccc1	dichloromethane	-6.14	-9.99	-10.64
N-methylpyrrole	Cn1ccccc1	dichloromethane	-5.80	-10.37	-10.37
N-methylpyrazole	Cn1cccn1	dichloromethane	-6.22	-10.16	-10.57
N-methylimidazole	Cn1ccnc1	dichloromethane	-8.06	-13.99	-13.78
N-methylaniline	CNc1ccccc1	dichloromethane	-7.86	-12.55	-13.79
N,N-dimethylaniline	CN(C)c1ccccc1	dichloromethane	-7.87	-12.90	-13.88
pyridine	c1ccncc1	dichloromethane	-6.46	-10.11	-10.74
3-methylpyridine	Cc1ccncc1	dichloromethane	-7.34	-11.42	-12.30
4-methylpyridine	Cc1ccncc1	dichloromethane	-7.34	-11.50	-12.28
acetophenone	CC(=O)c1ccccc1	dichloromethane	-8.24	-13.75	-13.71
methyl benzoate	COC(=O)c1ccccc1	dichloromethane	-8.48	-13.62	-14.10
ethyl benzoate	CCOC(=O)c1ccccc1	dichloromethane	-9.07	-14.36	-15.12
propyl benzoate	CCCOC(=O)c1ccccc1	dichloromethane	-9.66	-15.78	-16.16
butyl benzoate	CCCCOC(=O)c1ccccc1	dichloromethane	-10.38	-16.72	-17.36
methyl 2-hydroxybenzoate	COC(=O)c1ccccc1O	dichloromethane	-9.56	-13.47	-16.46
methyl 4-hydroxybenzoate	COC(=O)c1ccc(O)cc1	dichloromethane	-10.84	-15.65	-18.85
2-methoxyphenol	COc1ccccc1O	dichloromethane	-8.99	-13.82	-16.30
4-methoxyphenol	COc1ccc(O)cc1	dichloromethane	-9.54	-15.11	-16.83
2-chlorophenol	Oc1ccccc1Cl	dichloromethane	-7.49	-11.43	-12.58
4-chlorophenol	Oc1ccc(Cl)cc1	dichloromethane	-8.16	-13.16	-13.90
dimethyl sulfoxide	C[S](C)=O	dichloromethane	-8.02	-14.17	-14.20

tetrahydrothiophene	C1CCSC1	dichloromethane		-5.56	-9.76	-9.21
tetramethylstannane	C[Sn](C)(C)C	dichloromethane		-4.08	-6.38	-6.83
methane	C	methanol		0.32	-0.86	-0.99
ethane	CC	methanol		-0.31	-1.90	-1.88
isobutane	CC(C)C	methanol		-1.50	-3.91	-3.73
butane	CCCC	methanol		-1.65	-4.49	-3.96
pentane	CCCCC	methanol		-2.29	-5.35	-4.99
hexane	CCCCCC	methanol		-2.89	-6.34	-5.94
heptane	CCCCCCC	methanol		-3.49	-7.35	-6.89
octane	CCCCCCCC	methanol		-4.15	-8.34	-8.04
nonane	CCCCCCCCC	methanol		-4.83	-9.28	-9.06
decane	CCCCCCCCC	methanol		-5.52	-10.23	-10.17
dodecane	CCCCCCCCCCC	methanol		-6.83	-12.21	-12.39
tetradecane	CCCCCCCCCCCCC	methanol		-8.12	-14.22	-14.50
hexadecane	CCCCCCCCCCCCCCC	methanol		-9.43	-16.25	-16.57
2,2-dimethylbutane	CCC(C)(C)C	methanol		-2.45	-5.56	-5.38
3-ethylpentane	CCC(CC)CC	methanol		-3.20	-7.20	-6.44
2-methyloctane	CCCCCCC(C)C	methanol		-4.59	-9.01	-8.74
cyclopentane	C1CCCC1	methanol		-2.79	-5.88	-5.52
cycloheptane	C1CCCCC1	methanol		-4.15	-7.85	-7.73
cyclooctane	C1CCCCCCC1	methanol		-4.77	-8.82	-8.73
cis-1,2-dimethylcyclohexane	C[C@H]1CCCC[C@H]1C	methanol		-4.41	-8.21	-8.14
bicyclohexyl	C1CCC(CC1)C2CCCCC2	methanol		-7.28	-11.92	-12.09
adamantane	C1C2CC3CC1CC(C2)C3	methanol		-6.47	-10.11	-10.30
1-butene	CCC=C	methanol		-2.08	-4.59	-4.58
cis-2-butene	C/C=C/C	methanol		-2.19	-4.95	-4.78
1-pentene	CCCC=C	methanol		-2.74	-5.60	-5.61
1-hexene	CCCCC=C	methanol		-3.32	-6.65	-6.53
1-heptene	CCCCC=C	methanol		-3.84	-7.61	-7.35
1-octene	CCCCC=C	methanol		-4.42	-8.56	-8.27
1-nonene	CCCCC=C	methanol		-5.07	-9.55	-9.32
1-dodecene	CCCCCCCCC=C	methanol		-7.06	-12.57	-12.72
1-tridecene	CCCCCCCCCCC=C	methanol		-7.81	-13.52	-13.89
1-tetradecene	CCCCCCCCCCCC=C	methanol		-8.39	-14.55	-14.77
1-pentadecene	CCCCCCCCCCCCC=C	methanol		-9.04	-15.58	-15.97
cis-2-octene	CCCC/C=C/C	methanol		-4.50	-8.36	-8.45
trans-2-octene	CCCC/C=C/C	methanol		-4.43	-8.35	-8.32
trans-4-octene	CCC/C=C/CCC	methanol		-4.55	-8.22	-8.47
1,3-butadiene	C=CC=C	methanol		-2.52	-5.14	-5.23
1,5-hexadiene	C=CCCC=C	methanol		-3.86	-6.96	-7.34
cyclopentene	C1CC=CC1	methanol		-3.24	-6.08	-6.33
cyclooctene	C1CCCC=CC1	methanol		-4.59	-8.78	-8.26
1,3-cyclopentadiene	C1C=CC=C1	methanol		-3.44	-6.39	-6.65
1,4-cyclohexadiene	C1C=CCC=C1	methanol		-4.18	-7.61	-7.76
1,5-cyclooctadiene	C1CC=CCCC=C1	methanol		-5.31	-9.63	-9.44
1,3,5-cycloheptatriene	C1C=CC=CC=C1	methanol		-5.00	-8.97	-8.99
cyclooctatetraene	C1=CC=CC=CC1	methanol		-5.71	-9.98	-10.02
methanol	CO	methanol		-3.67	-9.03	-8.41
ethanol	CCO	methanol		-4.24	-10.11	-9.46
butan-1-ol	CCCCO	methanol		-5.29	-12.23	-11.21
octan-1-ol	CCCCCCCCO	methanol		-8.13	-16.11	-15.83
decan-1-ol	CCCCCCCCCO	methanol		-9.37	-18.28	-17.88
2-methyl-2-butanol	CCC(C)(C)O	methanol		-5.02	-12.47	-10.96
3-methyl-1-butanol	CC(C)CCO	methanol		-5.93	-13.01	-12.21
ethylene glycol	OCCO	methanol		-6.22	-15.52	-14.54
1,2-propanediol	CC(O)CO	methanol		-6.58	-15.46	-15.35
1,4-butanediol	OCCCCO	methanol		-8.57	-18.21	-18.10
2-butoxyethanol	CCCCOCCO	methanol		-7.41	-13.63	-14.78
benzene	c1ccccc1	methanol		-4.23	-7.74	-7.84
toluene	Cc1ccccc1	methanol		-4.76	-8.45	-8.67
isopropylbenzene	CC(C)c1ccccc1	methanol		-5.87	-10.12	-10.39
4-isopropyltoluene	CC(C)c1ccc(C)cc1	methanol		-6.42	-11.13	-11.27
sec-butylbenzene	CCC(C)c1ccccc1	methanol		-6.54	-11.17	-11.48
hexamethylbenzene	Cc1c(C)c(C)c(C)c(C)c1C	methanol		-7.42	-14.88	-13.13
octylbenzene	CCCCCCCCc1ccccc1	methanol		-9.22	-14.43	-15.79
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	methanol		-5.75	-11.10	-10.20
naphthalene	c1ccc2ccccc2c1	methanol		-7.19	-12.86	-12.32
biphenyl	c1ccc(cc1)c2ccccc2	methanol		-8.74	-14.78	-14.54
chloroform	ClC(Cl)Cl	methanol		-4.21	-8.63	-8.03
2-chloro-2-methylpropane	CC(C)(C)Cl	methanol		-3.32	-6.56	-6.35
2-methyl-2-bromopropane	CC(C)(C)Br	methanol		-3.45	-6.88	-6.63
2-methyl-2-iodopropane	CC(C)(C)I	methanol		-4.59	-7.84	-8.02
1,1-difluoroethane	CC(F)F	methanol		-2.31	-4.53	-4.48
methyl ethyl ketone	CCC(C)=O	methanol		-4.30	-7.71	-7.75
2-pentanone	CCCC(C)=O	methanol		-4.83	-8.57	-8.63
2-hexanone	CCCCC(C)=O	methanol		-5.32	-9.59	-9.41
3-hexanone	CCCC(=O)CC	methanol		-5.28	-9.43	-9.35
2-heptanone	CCCCC(C)=O	methanol		-5.99	-10.59	-10.53
4-heptanone	CCCC(=O)CCC	methanol		-5.86	-10.33	-10.30
2-octanone	CCCCC(C)=O	methanol		-6.66	-11.53	-11.61
2-nonanone	CCCCCCC(C)=O	methanol		-7.25	-12.40	-12.62
5-nonanone	CCCCC(=O)CCCC	methanol		-7.12	-12.18	-12.43
2-decanone	CCCCCCCC(C)=O	methanol		-7.86	-13.21	-13.67



2-undecanone	CCCCCCCCC(C)=O	methanol	-8.39	-14.10	-14.45
methyl isobutyl ketone	CC(C)CC(C)=O	methanol	-5.21	-9.47	-9.32
di- <i>tert</i> -butylketone	CC(C)(C)C(=O)C(C)C	methanol	-5.65	-9.92	-10.40
cyclopentanone	O=C1CCCC1	methanol	-5.43	-9.38	-9.53
cyclohexanone	O=C1CCCCC1	methanol	-6.02	-10.63	-10.44
cycloheptanone	O=C1CCCCC1	methanol	-6.67	-11.15	-11.53
diethyl ether	CCOCC	methanol	-3.30	-6.41	-6.28
diisopropyl ether	CC(C)OC(C)C	methanol	-4.14	-7.86	-7.91
butyl methyl ether	CCCCOC	methanol	-3.91	-7.32	-7.32
methyl <i>tert</i> -butyl ether	COC(C)(C)C	methanol	-3.51	-7.35	-6.88
methyl <i>tert</i> -amyl ether	CCC(C)(C)OC	methanol	-4.03	-8.30	-7.81
tetrahydrofuran	C1CCOC1	methanol	-3.81	-7.40	-6.93
tetrahydropyran	C1CCOCC1	methanol	-4.32	-8.00	-7.71
1,4-dioxane	C1COCCO1	methanol	-4.95	-8.32	-8.91
1,2-dimethoxyethane	COCCOC	methanol	-4.89	-8.72	-8.86
12-crown-4	C1COCCOCCOCCO1	methanol	-8.80	-15.56	-16.77
18-crown-6	C1COCCOCCOCCOCCOCCO1	methanol	-12.07	-24.28	-23.35
aniline	Nc1ccccc1	methanol	-7.36	-14.14	-12.97
nitric oxide	[N]=O	methanol	0.57	-0.63	-0.52
helium	[He]	methanol	2.01	1.40	2.00
neon	[Ne]	methanol	1.88	1.15	1.75
argon	[Ar]	methanol	0.97	-0.20	0.19
krypton	[Kr]	methanol	0.39	-1.17	-0.54
xenon	[Xe]	methanol	-0.69	-2.25	-2.38
radon	[Rn]	methanol	-0.85	-3.82	-2.57
nitrogen	N#N	methanol	1.01	0.12	0.35
carbon dioxide	O=C=O	methanol	-1.05	-2.55	-3.56
oxygen	O=O	methanol	0.96	-0.23	-0.05
methyl formate	COC=O	methanol	-3.55	-5.85	-6.45
methyl acetate	COC(C)=O	methanol	-4.16	-6.94	-7.40
ethyl acetate	CCOC(C)=O	methanol	-4.49	-7.59	-7.97
butyl acetate	CCCCOC(C)=O	methanol	-5.14	-9.55	-9.14
ethyl isobutyrate	CCOC(=O)C(C)C	methanol	-4.99	-8.70	-8.95
methyl pentanoate	CCCCC(=O)OC	methanol	-5.19	-9.47	-9.13
ethyl lactate	CCOC(=O)C(C)O	methanol	-7.11	-12.90	-14.55
acetonitrile	CC#N	methanol	-4.48	-6.84	-7.20
1-butylamine	CCCCN	methanol	-4.90	-12.17	-10.48
sec-butylamine	CCC(C)N	methanol	-4.11	-11.83	-9.79
<i>tert</i> -butylamine	CC(C)(C)N	methanol	-4.15	-11.83	-10.18
1-hexylamine	CCCCCCN	methanol	-5.50	-14.22	-11.86
1-heptylamine	CCCCCCCN	methanol	-6.55	-15.08	-13.55
dipropylamine	CCCNCCC	methanol	-5.38	-13.58	-11.85
dibutylamine	CCCCNCCCC	methanol	-6.14	-14.94	-13.35
triethylamine	CCN(CC)CC	methanol	-4.14	-11.42	-8.95
tripropylamine	CCCN(CCC)CCC	methanol	-5.73	-12.45	-11.94
cyclohexylamine	NC1CCCCC1	methanol	-6.18	-13.79	-12.46
chlorobenzene	Clc1ccccc1	methanol	-5.32	-9.61	-9.35
1,2-dichlorobenzene	Clc1ccccc1Cl	methanol	-6.38	-11.06	-11.13
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	methanol	-6.60	-11.02	-11.24
fluorobenzene	Fc1ccccc1	methanol	-4.70	-8.46	-8.57
bromobenzene	Brc1ccccc1	methanol	-5.53	-10.17	-9.58
iodobenzene	Ic1ccccc1	methanol	-6.40	-11.35	-10.52
nitromethane	C[N+](=[O-])=O	methanol	-4.64	-8.11	-8.65
4-nitrophenol	Oc1ccc(cc1)[N+](=[O-])=O	methanol	-10.80	-21.79	-19.50
4-bromophenol	Oc1ccc(Br)cc1	methanol	-9.56	-19.79	-17.51
phenol	Oc1ccccc1	methanol	-7.61	-15.78	-14.30
4- <i>tert</i> -butylphenol	CC(C)(C)c1ccc(O)cc1	methanol	-9.63	-18.72	-17.63
pyridine	c1ccncc1	methanol	-5.70	-10.57	-9.45
2-methylpyridine	Cc1cccn1	methanol	-6.25	-11.56	-10.51
3-methylpyridine	Cc1cccn1	methanol	-6.30	-11.90	-10.52
4-ethylpyridine	CCc1ccncc1	methanol	-6.96	-12.14	-11.61
2,6-dimethylpyridine	Cc1ccccc1n1	methanol	-7.02	-12.64	-12.05
3-chloropyridine	Clc1ccncc1	methanol	-7.35	-11.85	-11.96
4-cyanopyridine	N#Cc1ccncc1	methanol	-8.90	-12.43	-13.20
4-methoxypyridine	COc1ccncc1	methanol	-8.09	-13.52	-13.45
ethyl benzoate	CCOC(=O)c1ccccc1	methanol	-8.09	-12.89	-13.46
propyl benzoate	CCCOC(=O)c1ccccc1	methanol	-8.74	-14.20	-14.64
butyl benzoate	CCCCOC(=O)c1ccccc1	methanol	-9.49	-15.11	-15.90
1,2-dinitrobenzene	[O-][N+](=O)c1ccccc1[N+](=[O-])=O	methanol	-8.93	-15.31	-15.34
1,4-dinitrobenzene	[O-][N+](=O)c1ccc(cc1)[N+](=[O-])=O	methanol	-10.29	-16.79	-17.52
1-chloro-2-nitrobenzene	[O-][N+](=O)c1ccccc1Cl	methanol	-7.73	-14.62	-13.08
1-chloro-4-nitrobenzene	[O-][N+](=O)c1ccc(Cl)cc1	methanol	-8.67	-13.65	-14.46
acetophenone	CC(=O)c1ccccc1	methanol	-7.34	-11.56	-12.18
2-nitrophenol	Oc1ccccc1[N+](=[O-])=O	methanol	-8.67	-12.72	-15.30
3-nitrophenol	Oc1cccc(c1)[N+](=[O-])=O	methanol	-10.72	-21.05	-19.38
anisole	COc1ccccc1	methanol	-5.95	-10.34	-10.17
benzonitrile	N#Cc1ccccc1	methanol	-8.43	-11.64	-13.19
3-methylaniline	Cc1cccc(N)c1	methanol	-7.98	-14.57	-14.16
2-nitroaniline	Nc1ccccc1[N+](=[O-])=O	methanol	-10.75	-17.07	-19.12
3-nitroaniline	Nc1cccc(c1)[N+](=[O-])=O	methanol	-11.11	-18.66	-19.95
4-nitroaniline	Nc1ccc(cc1)[N+](=[O-])=O	methanol	-11.08	-20.66	-19.79

1,2-diphenylethane	C(Cc1ccccc1)c2ccccc2	methanol	-10.35	-15.94	-17.04
N,N-dimethylaniline	CN(C)c1ccccc1	methanol	-7.01	-11.60	-12.65
1-chloronaphthalene	Clc1ccccc2ccccc12	methanol	-8.29	-14.75	-13.84
1-nitronaphthalene	[O-][N+](=O)c1ccccc2ccccc12	methanol	-10.43	-17.42	-17.14
1-naphthylamine	Nc1ccccc2ccccc12	methanol	-10.78	-18.76	-18.69
$\alpha$ -methylstyrene	CC(=C)c1ccccc1	methanol	-6.04	-11.11	-10.54
trans-stilbene	c1ccc(cc1)/C=C/c2ccccc2	methanol	-10.39	-17.90	-17.05
diphenyl ether	O(c1ccccc1)c2ccccc2	methanol	-9.76	-14.90	-15.89
1-naphthol	Oc1ccccc2ccccc12	methanol	-10.87	-19.95	-19.44
quinoline	c1ccc2ncccc2c1	methanol	-9.28	-14.42	-15.20
pyrrole	[nH]1ccccc1	methanol	-5.91	-11.11	-10.74
N-methylpyrrole	Cn1ccccc1	methanol	-5.09	-8.92	-9.48
salicylamide	NC(=O)c1ccccc1O	methanol	-10.66	-18.80	-18.85
2,2,2-trifluoroethanol	OCC(F)(F)F	methanol	-4.52	-11.26	-11.19
benzamide	NC(=O)c1ccccc1	methanol	-10.98	-20.33	-19.23
benzoic acid	OC(=O)c1ccccc1	methanol	-9.39	-18.41	-17.39
picric acid	Oc1c(cc(c1[N+](=O)[O-])=O)[N+](=O)[O-]	methanol	-13.98	-22.84	-24.80
tetramethylsilane	C[Si](C)(C)C	methanol	-2.94	-5.00	-5.51
tetraethyltin	CC[Sn](CC)(CC)CC	methanol	-5.61	-10.23	-9.63
formamide	NC=O	methanol	-7.24	-14.36	-14.20
dimethylformamide	CN(C)C=O	methanol	-5.81	-11.47	-11.09
pyrrolidine	C1CCNC1	methanol	-5.60	-12.17	-11.15
N-methylpyrrolidine	CN1CCCC1	methanol	-4.61	-10.57	-8.92
piperidine	C1CCNCC1	methanol	-6.11	-12.60	-12.12
N-methylpiperidine	CN1CCCCC1	methanol	-5.12	-11.28	-9.89
water	O	methanol	-4.19	-11.23	-10.33
imidazole	[nH]1ccnc1	methanol	-8.99	-16.32	-16.13
2-methylimidazole	Cc1[nH]ccn1	methanol	-9.31	-17.90	-16.60
2-ethylimidazole	CCc1[nH]ccn1	methanol	-9.83	-17.83	-17.39
2-isopropylimidazole	CC(C)c1[nH]ccn1	methanol	-10.33	-19.02	-18.44
pyrazole	[nH]1cccn1	methanol	-7.44	-13.46	-13.65
3,5-dimethylpyrazole	CC1=CC(C)=NN1	methanol	-8.71	-15.56	-16.26
3,4,5-trimethylpyrazole	Cc1[nH]nc(C)c1C	methanol	-9.17	-18.55	-17.13
tetramethylstannane	C[Sn](C)(C)C	methanol	-3.57	-6.75	-6.39
N-methylimidazole	Cn1ccnc1	methanol	-6.95	-14.70	-11.70
methane	C	ethanol	0.39	-0.92	-0.92
ethane	CC	ethanol	-0.37	-2.10	-2.05
butane	CCCC	ethanol	-1.74	-4.91	-4.19
pentane	CCCCC	ethanol	-2.38	-5.97	-5.21
heptane	CCCCCCC	ethanol	-3.76	-8.00	-7.45
octane	CCCCCCCC	ethanol	-4.45	-8.21	-8.65
decane	CCCCCCCCC	ethanol	-5.80	-11.31	-10.73
undecane	CCCCCCCCCC	ethanol	-6.46	-12.09	-11.90
dodecane	CCCCCCCCCCC	ethanol	-7.18	-13.19	-13.10
3-ethylpentane	CCC(CC)CC	ethanol	-3.47	-7.75	-6.99
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	ethanol	-3.66	-7.72	-7.49
cyclopentane	C1CCCC1	ethanol	-2.96	-6.34	-5.85
cyclooctane	C1CCCCCCC1	ethanol	-5.02	-9.53	-9.23
adamantane	C1C2CC3CC1CC(C2)C3	ethanol	-6.50	-10.76	-10.36
1-heptene	CCCCCC=C	ethanol	-4.01	-8.02	-7.73
2,4,4-trimethyl-1-pentene	CC(=C)CC(C)(C)C	ethanol	-3.90	-7.92	-7.69
1-octyne	CCCCCCC#C	ethanol	-5.02	-9.78	-9.25
2-octyne	CCCCC#CC	ethanol	-4.99	-9.96	-9.13
methanol	CO	ethanol	-3.69	-8.94	-8.50
ethanol	CCO	ethanol	-4.26	-10.11	-9.55
butan-1-ol	CCCCO	ethanol	-5.48	-12.39	-11.61
hexan-1-ol	CCCCCO	ethanol	-6.86	-14.34	-13.93
decan-1-ol	CCCCCCCCCO	ethanol	-9.55	-18.86	-18.23
isopropanol	CC(C)O	ethanol	-4.56	-10.87	-10.13
3-methyl-1-butanol	CC(C)CCO	ethanol	-6.13	-13.28	-12.60
2-methyl-2-butanol	CC(C)(C)O	ethanol	-5.06	-12.55	-11.00
2-butoxyethanol	CCCCOCCO	ethanol	-7.39	-13.40	-14.68
dimethyl ether	COC	ethanol	-2.05	-3.91	-4.23
diethyl ether	CCOCC	ethanol	-3.16	-6.13	-6.03
dibutyl ether	CCCCOCCCC	ethanol	-5.67	-10.04	-10.29
methyl butyl ether	CCCCOC	ethanol	-3.82	-7.26	-7.15
diisopropyl ether	CC(C)OC(C)C	ethanol	-4.10	-7.64	-7.85
methyl tert-amyl ether	CCC(C)(C)OC	ethanol	-3.95	-8.27	-7.66
tetrahydrofuran	C1CCOC1	ethanol	-3.69	-7.28	-6.70
tetrahydropyran	C1CCOCC1	ethanol	-4.24	-7.79	-7.56
1,2-diethoxyethane	CCOCCOCC	ethanol	-5.72	-9.99	-10.21
18-crown-6	C1COCCOCCOCCOCCOCCO1	ethanol	-11.92	-21.53	-23.03
nitric oxide	[N]=O	ethanol	0.53	-1.08	-0.64
helium	[He]	ethanol	2.04	1.73	2.07
neon	[Ne]	ethanol	1.88	0.93	1.74
argon	[Ar]	ethanol	0.96	-0.09	0.17
xenon	[Xe]	ethanol	-0.69	-2.26	-2.43
radon	[Rn]	ethanol	-0.87	-2.84	-2.67
hydrogen	[H][H]	ethanol	1.57	0.89	1.11
nitrogen	N#N	ethanol	0.99	0.11	0.29
oxygen	O=O	ethanol	1.09	-0.29	0.12
carbon monoxide	C=O	ethanol	0.62	0.08	-0.51

carbon dioxide	O=C=O	ethanol	-0.86	-3.06	-3.28
nitromethane	C[N+](=O)=O	ethanol	-4.44	-7.65	-8.32
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	ethanol	-7.88	-13.23	-12.93
butylamine	CCCCN	ethanol	-5.10	-11.31	-10.88
1-heptylamine	CCCCCCCN	ethanol	-6.71	-14.60	-13.84
dibutylamine	CCCCNCCCC	ethanol	-6.30	-14.56	-13.61
triethylamine	CCN(CC)CC	ethanol	-4.29	-10.52	-9.19
tripropylamine	CCCN(CCC)CCC	ethanol	-5.82	-11.74	-12.07
tributylamine	CCCCN(CCCC)CCCC	ethanol	-7.49	-15.58	-14.97
dimethyl carbonate	COC(=O)OC	ethanol	-4.38	-7.26	-7.70
diethyl carbonate	CCOC(=O)OCC	ethanol	-4.81	-9.05	-8.46
methyl isobutyl ketone	CC(C)CC(C)=O	ethanol	-5.17	-9.02	-9.26
cyclohexanone	O=C1CCCCC1	ethanol	-6.07	-9.80	-10.54
aniline	Nc1ccccc1	ethanol	-7.48	-13.68	-13.23
ethyl formate	CCOC=O	ethanol	-3.69	-6.60	-6.65
methyl acetate	COC(C)=O	ethanol	-3.93	-6.66	-6.99
ethyl acetate	CCOC(C)=O	ethanol	-4.25	-7.28	-7.56
propyl acetate	CCCOC(C)=O	ethanol	-4.64	-8.27	-8.25
butyl acetate	CCCCOC(C)=O	ethanol	-5.16	-9.28	-9.16
pentyl acetate	CCCCCOC(C)=O	ethanol	-5.84	-10.56	-10.33
methyl propanoate	CCC(=O)OC	ethanol	-4.10	-7.30	-7.24
methyl butanoate	CCCC(=O)OC	ethanol	-4.57	-8.60	-8.07
methyl pentanoate	CCCCC(=O)OC	ethanol	-5.20	-9.13	-9.14
ethyl isobutyrate	CCOC(=O)C(C)C	ethanol	-4.99	-8.24	-8.94
methyl benzoate	COC(=O)c1ccccc1	ethanol	-7.41	-12.05	-12.23
ethyl benzoate	CCOC(=O)c1ccccc1	ethanol	-8.10	-13.15	-13.47
propyl benzoate	CCCOC(=O)c1ccccc1	ethanol	-8.75	-13.98	-14.66
butyl benzoate	CCCCOC(=O)c1ccccc1	ethanol	-9.53	-14.99	-15.99
methyl lactate	COC(=O)C(C)O	ethanol	-6.90	-12.19	-14.09
ethyl lactate	CCOC(=O)C(C)O	ethanol	-7.01	-12.78	-14.37
acetonitrile	CC#N	ethanol	-4.36	-6.49	-7.01
tetrachloromethane	ClC(Cl)(Cl)Cl	ethanol	-4.21	-7.93	-8.14
chloroform	ClC(Cl)Cl	ethanol	-4.20	-8.82	-8.06
2-chloro-2-methylbutane	CCC(C)(C)Cl	ethanol	-4.03	-7.83	-7.53
2-chloro-2-methylpentane	CCCC(C)(C)Cl	ethanol	-4.65	-9.03	-8.54
2-methyl-2-bromobutane	CCC(C)(C)Br	ethanol	-4.10	-8.48	-7.78
dimethyl sulfoxide	C[S](C)=O	ethanol	-6.98	-11.76	-12.09
morpholine	C1COCCN1	ethanol	-7.38	-12.46	-14.02
pyridine	c1ccncc1	ethanol	-5.59	-10.38	-9.27
4-ethylpyridine	CCc1ccncc1	ethanol	-7.02	-11.66	-11.74
quinoline	c1ccc2ncccc2c1	ethanol	-9.27	-14.36	-15.19
2,2,2-trifluoroethanol	OCC(F)(F)F	ethanol	-4.59	-11.52	-11.40
benzene	c1ccccc1	ethanol	-4.14	-7.69	-7.68
toluene	Cc1ccccc1	ethanol	-4.73	-8.46	-8.62
ethylbenzene	CCc1ccccc1	ethanol	-5.38	-9.67	-9.61
1,4-dimethylbenzene	Cc1ccc(C)cc1	ethanol	-5.31	-9.54	-9.53
chlorobenzene	Clc1ccccc1	ethanol	-5.28	-9.72	-9.30
ammonia	N	ethanol	-2.65	-6.27	-5.85
dichlorodifluoromethane	FC(F)(Cl)Cl	ethanol	-1.63	-4.22	-4.61
pentafluoroethane	FC(F)C(F)(F)F	ethanol	-1.87	-3.95	-3.87
chloropentafluoroethane	FC(F)(F)C(F)(F)Cl	ethanol	-0.51	-3.00	-2.78
imidazole	[nH]1ccnc1	ethanol	-9.15	-17.56	-16.50
formamide	NC=O	ethanol	-7.16	-13.98	-14.15
methylformamide	CNC=O	ethanol	-6.71	-12.50	-12.96
dimethylformamide	CN(C)C=O	ethanol	-5.73	-10.70	-10.95
benzamide	NC(=O)c1ccccc1	ethanol	-11.04	-19.78	-19.40
benzoic acid	OC(=O)c1ccccc1	ethanol	-9.51	-18.29	-17.66
benzaldehyde	O=Cc1ccccc1	ethanol	-6.59	-10.88	-10.95
adipic acid	OC(=O)CCCCC(O)=O	ethanol	-12.87	-26.10	-26.06
sebacic acid	OC(=O)CCCCCCCCC(O)=O	ethanol	-14.53	-30.74	-29.54
trifluoromethane	FC(F)F	ethanol	-0.82	-2.80	-2.49
carbon tetrafluoride	FC(F)(F)F	ethanol	0.96	-0.21	-0.46
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	ethanol	-9.76	-17.68	-17.30
ethylene carbonate	O=C1OCCO1	ethanol	-5.30	-8.39	-9.50
benzyl alcohol	OCc1ccccc1	ethanol	-8.75	-15.32	-16.39
trimethyl phosphate	CO[P](=O)(OC)OC	ethanol	-7.59	-10.17	-10.46
diethyl malonate	CCOC(=O)CC(=O)OCC	ethanol	-7.77	-12.13	-13.42
pimelic acid	OC(=O)CCCCCCC(O)=O	ethanol	-14.02	-27.68	-27.79
azelaic acid	OC(=O)CCCCCCCCC(O)=O	ethanol	-14.17	-30.76	-28.96
succinic acid	OC(=O)CCC(O)=O	ethanol	-11.63	-24.27	-23.47
N-methylimidazole	Cn1ccnc1	ethanol	-6.94	-13.86	-11.67
pentane	CCCCC	pentane	-3.24	-6.39	-6.05
methyl methacrylate	COC(=O)C(C)=C	pentane	-4.59	-7.69	-8.38
pentyl acetate	CCCCCOC(C)=O	pentane	-5.88	-10.51	-10.33
butyl acetate	CCCCOC(C)=O	pentane	-5.25	-9.58	-9.37
butyl propanoate	CCCCOC(=O)CC	pentane	-5.90	-10.56	-10.39
propyl acetate	CCCOC(C)=O	pentane	-4.66	-8.14	-8.53
ethyl butanoate	CCCC(=O)OCC	pentane	-5.32	-9.15	-9.55
ethyl pentanoate	CCCCC(=O)OCC	pentane	-5.89	-10.39	-10.36
ethyl hexanoate	CCCCCC(=O)OCC	pentane	-6.57	-11.64	-11.41
xenon	[Xe]	pentane	-1.24	-2.62	-2.65
propanenitrile	CCC#N	pentane	-3.75	-6.24	-6.53
acetophenone	CC(=O)c1ccccc1	pentane	-6.39	-10.74	-10.94

methyl acrylate	<chem>COC(=O)C=C</chem>	pentane	-3.98	-7.12	-7.49
1,1,1-trichloroethane	<chem>CC(Cl)(Cl)Cl</chem>	pentane	-4.60	-7.38	-7.99
methyl ethyl ketone	<chem>CCC(C)=O</chem>	pentane	-3.72	-6.64	-6.93
2-pentanone	<chem>CCCC(C)=O</chem>	pentane	-4.42	-7.77	-8.05
3-pentanone	<chem>CCC(=O)CC</chem>	pentane	-4.47	-7.91	-8.13
methane	<chem>C</chem>	hexane	-0.09	-0.54	-1.28
ethane	<chem>CC</chem>	hexane	-1.00	-1.99	-2.72
propane	<chem>CCC</chem>	hexane	-1.73	-3.37	-3.84
butane	<chem>CCCC</chem>	hexane	-2.44	-4.90	-4.92
pentane	<chem>CCCCC</chem>	hexane	-3.17	-6.39	-6.06
hexane	<chem>CCCCCC</chem>	hexane	-3.87	-7.54	-7.14
heptane	<chem>CCCCCCC</chem>	hexane	-4.60	-8.74	-8.29
octane	<chem>CCCCCCCC</chem>	hexane	-5.35	-9.92	-9.54
decane	<chem>CCCCCCCCC</chem>	hexane	-6.73	-12.15	-11.63
dodecane	<chem>CCCCCCCCCCCC</chem>	hexane	-8.15	-14.72	-13.92
hexadecane	<chem>CCCCCCCCCCCCCCCC</chem>	hexane	-10.86	-19.44	-18.07
isobutane	<chem>CC(C)C</chem>	hexane	-2.35	-4.51	-4.78
2,2-dimethylpropane	<chem>CC(C)(C)C</chem>	hexane	-2.92	-5.15	-5.78
2,4-dimethylpentane	<chem>CC(C)CC(C)C</chem>	hexane	-4.36	-7.81	-7.90
2,2,4-trimethylpentane	<chem>CC(C)CC(C)(C)C</chem>	hexane	-4.89	-8.42	-8.85
cyclohexane	<chem>C1CCCCC1</chem>	hexane	-4.11	-7.75	-7.29
adamantane	<chem>C1C2CC3CC1CC(C2)C3</chem>	hexane	-7.14	-11.57	-11.19
ethene	<chem>C=C</chem>	hexane	-0.96	-1.78	-2.65
benzene	<chem>c1ccccc1</chem>	hexane	-4.15	-7.34	-7.64
naphthalene	<chem>c1ccc2ccccc2c1</chem>	hexane	-6.89	-12.24	-11.82
chlorobenzene	<chem>Clc1ccccc1</chem>	hexane	-5.17	-9.09	-9.10
1,2-dichlorobenzene	<chem>Clc1ccccc1Cl</chem>	hexane	-6.01	-10.60	-10.29
nitrobenzene	<chem>[O-][N+](=O)c1ccccc1</chem>	hexane	-5.68	-9.67	-10.11
ethanol	<chem>CCO</chem>	hexane	-2.23	-4.61	-4.75
1-propanol	<chem>CCCO</chem>	hexane	-2.95	-5.27	-5.91
1-butanol	<chem>CCCCO</chem>	hexane	-3.68	-6.83	-7.10
2-ethyl-1-butanol	<chem>CCC(CC)CO</chem>	hexane	-4.94	-8.23	-9.13
1-decanol	<chem>CCCCCCCCCCO</chem>	hexane	-8.55	-15.14	-14.83
1,1,1,3,3,3-hexafluoro-isopropanol	<chem>OC(C(F)(F)F)C(F)(F)F</chem>	hexane	-1.81	-4.79	-5.12
benzaldehyde	<chem>O=Cc1ccccc1</chem>	hexane	-5.54	-9.77	-9.62
2-methylpyridine	<chem>Cc1cccn1</chem>	hexane	-5.45	-8.78	-9.38
3-methylpyridine	<chem>Cc1ccncc1</chem>	hexane	-5.50	-9.06	-9.46
4-methylpyridine	<chem>Cc1ccncc1</chem>	hexane	-5.49	-9.05	-9.44
2,4-dimethylpyridine	<chem>Cc1cnc(C)c1</chem>	hexane	-6.10	-9.93	-10.40
2,6-dimethylpyridine	<chem>Cc1cc(C)n1</chem>	hexane	-6.04	-9.60	-10.33
3-chloropyridine	<chem>Clc1cccn1</chem>	hexane	-6.04	-10.04	-10.33
3-cyanopyridine	<chem>N#Cc1cccn1</chem>	hexane	-6.35	-9.66	-10.17
4-cyanopyridine	<chem>N#Cc1ccncc1</chem>	hexane	-6.21	-9.32	-9.87
methyl methacrylate	<chem>COC(=O)C(C)=C</chem>	hexane	-4.43	-7.94	-8.13
propionitrile	<chem>CCC#N</chem>	hexane	-3.46	-5.76	-5.96
acetone	<chem>CC(C)=O</chem>	hexane	-2.73	-5.22	-5.34
2-pentanone	<chem>CCCC(C)=O</chem>	hexane	-4.28	-7.77	-7.81
3-pentanone	<chem>CCC(=O)CC</chem>	hexane	-4.33	-7.91	-7.90
dipropyl ether	<chem>CCCOCC</chem>	hexane	-4.62	-8.38	-8.28
butyl methyl ether	<chem>CCCCOC</chem>	hexane	-4.05	-7.48	-7.47
methyl tert-butyl ether	<chem>COC(C)(C)C</chem>	hexane	-3.52	-6.97	-6.55
ethyl tert-butyl ether	<chem>CCOC(C)(C)C</chem>	hexane	-4.07	-7.77	-7.38
methyl tert-amyl ether	<chem>CCC(C)(C)OC</chem>	hexane	-4.17	-8.32	-7.59
furan	<chem>c1ccoc1</chem>	hexane	-3.54	-5.70	-6.71
tetrahydropyran	<chem>C1CCOCC1</chem>	hexane	-4.63	-7.78	-8.45
dimethoxymethane	<chem>COCOC</chem>	hexane	-3.12	-5.70	-5.99
1,2-dimethoxyethane	<chem>COCOC</chem>	hexane	-3.94	-7.50	-7.23
paraldehyde	<chem>CC1OC(C)OC(C)O1</chem>	hexane	-5.50	-8.28	-9.74
acetal	<chem>CCOC(C)OCC</chem>	hexane	-4.74	-8.97	-8.51
methyl acetate	<chem>COC(C)=O</chem>	hexane	-3.22	-5.11	-6.27
propyl acetate	<chem>CCOC(C)=O</chem>	hexane	-4.47	-7.99	-8.19
butyl acetate	<chem>CCCCOC(C)=O</chem>	hexane	-5.09	-9.18	-9.15
ethyl propionate	<chem>CCOC(=O)CC</chem>	hexane	-4.53	-7.77	-8.30
ethyl hexanoate	<chem>CCCCC(=O)OCC</chem>	hexane	-6.46	-11.29	-11.30
propyl propionate	<chem>CCOC(=O)CC</chem>	hexane	-5.10	-9.00	-9.19
methyl decanoate	<chem>CCCCCCCCC(=O)OC</chem>	hexane	-8.62	-15.13	-14.63
helium	<chem>[He]</chem>	hexane	1.85	1.92	1.75
neon	<chem>[Ne]</chem>	hexane	1.72	1.30	1.41
xenon	<chem>[Xe]</chem>	hexane	-1.08	-2.56	-2.59
radon	<chem>[Rn]</chem>	hexane	-1.24	-3.03	-2.79
oxygen	<chem>O=O</chem>	hexane	0.77	-0.23	0.14
nitric oxide	<chem>[N]=O</chem>	hexane	0.39	-0.53	-0.44
tetrafluoromethane	<chem>FC(F)(F)F</chem>	hexane	0.40	-0.35	-0.75
sulfur hexafluoride	<chem>F[S](F)(F)(F)F</chem>	hexane	-0.38	-1.98	-1.85
triethylamine	<chem>CCN(CC)CC</chem>	hexane	-4.86	-8.26	-9.16
phenylamine	<chem>Nc1ccccc1</chem>	hexane	-5.70	-8.37	-9.91
hexylamine	<chem>CCCCCCN</chem>	hexane	-5.22	-9.71	-9.72
heptylamine	<chem>CCCCCCCN</chem>	hexane	-5.97	-10.90	-10.95
octylamine	<chem>CCCCCCCCN</chem>	hexane	-6.63	-12.11	-12.00
decylamine	<chem>CCCCCCCCCN</chem>	hexane	-7.96	-14.38	-14.29
nitromethane	<chem>C[N+](=O)[O-]</chem>	hexane	-2.34	-5.40	-4.95
nitroethane	<chem>CC[N+](=O)[O-]</chem>	hexane	-3.13	-6.60	-6.23

diethyl sulfide	CCSCC	hexane	-4.92	-8.04	-8.60
1,2-dichloroethane	ClCCCl	hexane	-3.68	-6.99	-6.66
chloroform	ClC(Cl)Cl	hexane	-3.59	-7.15	-6.47
ethyl iodide	CCl	hexane	-3.91	-6.85	-6.79
1-chlorobutane	CCCCl	hexane	-3.88	-8.18	-7.11
2-chloro-2-methylpropane	CC(C)(C)Cl	hexane	-3.59	-6.47	-6.72
1-chloronaphthalene	Clc1cccc2ccccc12	hexane	-7.90	-14.76	-13.24
acetophenone	CC(=O)c1ccccc1	hexane	-6.27	-10.70	-10.77
ethyl benzoate	CCOC(=O)c1ccccc1	hexane	-7.23	-12.93	-12.40
methyl benzoate	COC(=O)c1ccccc1	hexane	-6.64	-11.73	-11.47
tetramethylstannane	C[Sn](C)(C)C	hexane	-4.15	-7.40	-7.11
ethane	CC	heptane	-0.88	-2.67	-2.68
propane	CCC	heptane	-1.69	-4.09	-3.97
pentane	CCCCC	heptane	-3.18	-6.34	-6.30
hexane	CCCCCC	heptane	-3.89	-7.54	-7.38
heptane	CCCCCCC	heptane	-4.61	-8.74	-8.53
octane	CCCCCCCC	heptane	-5.37	-9.92	-9.78
nonane	CCCCCCCCC	heptane	-6.03	-11.09	-10.77
dodecane	CCCCCCCCCCCC	heptane	-8.15	-14.62	-14.13
hexadecane	CCCCCCCCCCCCCCCC	heptane	-10.86	-19.34	-18.30
2-methylpentane	CCCC(C)C	heptane	-3.78	-7.18	-7.20
3-methylpentane	CCC(C)CC	heptane	-3.77	-7.27	-7.20
2,2-dimethylbutane	CCC(C)(C)C	heptane	-3.61	-6.66	-7.05
2,3-dimethylbutane	CC(C)(C)C	heptane	-3.70	-7.00	-7.09
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	heptane	-4.88	-8.38	-9.04
cyclohexane	C1CCCCC1	heptane	-4.13	-7.72	-7.54
cycloheptane	C1CCCCC1	heptane	-4.84	-9.04	-8.67
cyclooctane	C1CCCCCCC1	heptane	-5.54	-10.20	-9.76
cyclodecane	C1CCCCCCCC1	heptane	-6.86	-12.45	-11.89
methylcyclopentane	CC1CCCC1	heptane	-4.03	-7.50	-7.37
methylcyclohexane	CC1CCCCC1	heptane	-4.70	-8.45	-8.39
cis-1,2-dimethylcyclohexane	C[C@H]1CCCC[C@H]1C	heptane	-5.27	-9.50	-9.26
trans-1,2-dimethylcyclohexane	C[C@H]1CCCC[C@@H]1C	heptane	-5.34	-9.25	-9.41
cis-decalin	C1CC[C@H]2CCCC[C@H]2C1	heptane	-6.95	-12.15	-11.61
trans-decalin	C1CC[C@H]2CCCC[C@@H]2C1	heptane	-6.90	-11.94	-11.52
bicyclohexyl	C1CCC(CC1)C2CCCCC2	heptane	-8.45	-13.82	-14.05
adamantane	C1C2CC3CC1CC(C2)C3	heptane	-7.08	-11.45	-11.22
1-hexene	CCCC=C	heptane	-3.91	-7.26	-7.45
1-octyne	CCCCCCC#C	heptane	-5.34	-9.57	-9.68
2-octyne	CCCCC#CC	heptane	-5.37	-10.19	-9.74
4-octyne	CCCC#CCCC	heptane	-5.36	-9.86	-9.72
propanal	CCC=O	heptane	-2.81	-4.83	-5.63
butanal	CCCC=O	heptane	-3.53	-6.02	-6.74
hexanal	CCCCC=O	heptane	-5.03	-8.71	-9.13
heptanal	CCCCC=O	heptane	-5.71	-9.94	-10.15
octanal	CCCCCCC=O	heptane	-6.42	-10.94	-11.41
nonanal	CCCCCCCC=O	heptane	-7.19	-12.15	-12.54
isobutyraldehyde	CC(C)C=O	heptane	-3.42	-6.29	-6.55
acetone	CC(C)=O	heptane	-2.70	-5.16	-5.44
methyl ethyl ketone	CCC(C)=O	heptane	-3.55	-6.34	-6.81
2-heptanone	CCCCC(C)=O	heptane	-5.65	-9.82	-10.11
3-heptanone	CCCC(=O)CC	heptane	-5.69	-10.02	-10.19
4-heptanone	CCCC(=O)CCC	heptane	-5.68	-9.92	-10.21
2-octanone	CCCCC(C)=O	heptane	-6.34	-10.93	-11.18
3-octanone	CCCCC(=O)CC	heptane	-6.30		-11.15
2-nonanone	CCCCCCC(C)=O	heptane	-7.02	-11.98	-12.26
3-nonanone	CCCCCCC(=O)CC	heptane	-6.98		-12.23
4-nonanone	CCCCC(=O)CCC	heptane	-6.99		-12.22
2-decanone	CCCCCCCC(C)=O	heptane	-7.64	-13.21	-13.23
4-decanone	CCCCCCC(=O)CCC	heptane	-7.63		-13.22
2-undecanone	CCCCCCCCC(C)=O	heptane	-8.31	-14.78	-14.24
3-undecanone	CCCCCCCCC(=O)CC	heptane	-8.30		-14.26
4-undecanone	CCCCCCCCC(=O)CCC	heptane	-8.33		-14.30
5-undecanone	CCCCCCCC(=O)CCCC	heptane	-8.27		-14.23
di-tert-butylketone	CC(C)(C)C(=O)C(C)(C)C	heptane	-5.59	-10.07	-9.89
cyclohexanone	O=C1CCCCC1	heptane	-5.25	-9.03	-9.31
butyl acetate	CCCCOC(C)=O	heptane	-5.05	-9.25	-9.24
pentyl acetate	CCCCCOC(C)=O	heptane	-5.71	-10.64	-10.28
hexyl acetate	CCCCCOC(C)=O	heptane	-6.34	-11.95	-11.25
nonyl acetate	CCCCCCCCCOC(C)=O	heptane	-8.33	-14.94	-14.38
butyl propionate	CCCCOC(=O)CC	heptane	-5.69	-10.74	-10.29
ethyl butanoate	CCCC(=O)OCC	heptane	-5.13	-9.10	-9.42
propyl butanoate	CCCOC(=O)CCC	heptane	-5.74	-10.30	-10.35
butyl butanoate	CCCCOC(=O)CCC	heptane	-6.35	-11.38	-11.29
methyl pentanoate	CCCCC(=O)OC	heptane	-5.14	-9.19	-9.39
methyl heptanoate	CCCCC(=O)OC	heptane	-6.44	-11.76	-11.45
methyl decanoate	CCCCCCCCC(=O)OC	heptane	-8.58	-15.13	-14.74
dimethyl oxalate	COC(=O)C(=O)OC	heptane	-5.01	-8.99	-9.41
dimethyl succinate	COC(=O)CCC(=O)OC	heptane	-6.20	-11.19	-11.22
dimethyl adipate	COC(=O)CCCCC(=O)OC	heptane	-7.21	-13.29	-12.74
dimethyl pimelate	COC(=O)CCCCC(=O)OC	heptane	-7.96	-14.72	-13.86

dimethyl suberate	COC(=O)CCCCCCC(=O)OC	heptane	-8.54	-15.94	-14.80
dimethyl azelate	COC(=O)CCCCCCCC(=O)OC	heptane	-9.21	-17.14	-15.74
methyl methacrylate	COC(=O)C(C)=C	heptane	-4.39	-7.91	-8.23
diethyl ether	CCOCC	heptane	-3.33	-5.81	-6.51
dibutyl ether	CCCCOCCCC	heptane	-5.94	-10.57	-10.52
dipentyl ether	CCCCCOCCCCC	heptane	-7.27	-12.56	-12.58
diisopropyl ether	CC(C)OC(C)C	heptane	-4.28	-7.40	-7.94
methyl heptyl ether	CCCCCCCOC	heptane	-6.08	-11.02	-10.74
methyl <i>tert</i> -butyl ether	COC(C)(C)C	heptane	-3.51	-5.93	-6.75
ethyl <i>tert</i> -butyl ether	CCOC(C)(C)C	heptane	-4.07	-7.72	-7.58
methyl <i>tert</i> -amyl ether	CCC(C)(C)OC	heptane	-4.17	-8.27	-7.78
2,5,8,11,14-pentaoxopentadecane	CC(=O)CCC(=O)CCC(=O)CCC(=O)CCC(C)=O	heptane	-11.56	-16.28	-19.08
2,5,8-trioxanonane	COCCOCCOC	heptane	-5.56	-9.55	-10.03
diethoxymethane	CCOCCOC	heptane	-4.33	-7.99	-7.97
1,2-dimethoxyethane	COCCOC	heptane	-3.96	-7.59	-7.45
dimethoxymethane	COCOC	heptane	-3.13	-6.23	-6.19
tetrahydrofuran	C1CCOC1	heptane	-3.88	-7.01	-7.38
2-methyltetrahydrofuran	CC1CCCOC1	heptane	-4.42	-7.55	-8.18
1-fluorooctane	CCCCCCCCF	heptane	-5.92	-11.44	-10.49
dichloromethane	CICCl	heptane	-2.81	-5.69	-5.56
trichloromethane	ClC(Cl)Cl	heptane	-3.61	-6.74	-6.73
tetrachloromethane	ClC(Cl)(Cl)Cl	heptane	-4.22	-7.46	-7.67
1-chlorobutane	CCCCCl	heptane	-3.91	-7.46	-7.37
1-chlorooctane	CCCCCCCCCl	heptane	-6.67	-12.16	-11.63
2-chloro-2-methylpropane	CC(C)(C)Cl	heptane	-3.52	-6.33	-6.72
1,2-dichloroethane	ClCCCl	heptane	-3.72	-6.69	-6.96
1,4-dichlorobutane	ClCCCCCl	heptane	-5.30	-9.89	-9.36
1,6-dichlorohexane	ClCCCCCCC1	heptane	-6.58	-12.00	-11.22
1,1-dichloropropane	CC(C)Cl	heptane	-4.33	-7.77	-7.85
1,2-dichloropropane	CC(Cl)CCl	heptane	-4.45	-7.84	-8.07
1,3-dichlorobutane	CC(Cl)CCC1	heptane	-5.21	-8.96	-9.16
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	heptane	-4.52	-7.19	-8.10
1,1,2,2-tetrachloroethane	ClC(Cl)(Cl)Cl	heptane	-5.52	-9.58	-9.48
chlorocyclohexane	ClC1CCCCC1	heptane	-5.56	-9.54	-9.76
1-bromopropane	CCCBBr	heptane	-3.70	-7.07	-7.17
1-bromobutane	CCCCBr	heptane	-4.30	-8.20	-8.05
1-bromopentane	CCCCCBr	heptane	-4.91	-9.35	-8.96
1-bromohexane	CCCCCCBr	heptane	-5.57	-10.44	-9.97
1-bromoheptane	CCCCCCCBr	heptane	-6.23	-11.57	-10.99
1-bromododecane	CCCCCCCCCCCCBr	heptane	-9.59	-17.45	-16.17
2-bromobutane	CCC(C)Br	heptane	-4.20	-7.65	-7.89
2-bromo-2-methylpropane	CC(C)(C)Br	heptane	-3.98	-6.98	-7.49
1,3-dibromopropane	BrCCBr	heptane	-5.63	-9.82	-9.98
1,4-dibromobutane	BrCCCCBr	heptane	-6.20	-11.02	-10.78
1,3-dibromobutane	CC(Br)CCBr	heptane	-6.14	-10.52	-10.69
1,12-dibromododecane	BrCCCCCCCCCCCCBr	heptane	-10.40		-16.90
1-iodopropane	CCCI	heptane	-4.44	-7.82	-7.74
1-iodobutane	CCCCI	heptane	-5.12	-9.01	-8.74
1-iodopentane	CCCCCI	heptane	-5.83	-10.21	-9.81
1-iodohexane	CCCCCCI	heptane	-6.55	-11.35	-10.93
2-iodopropane	CC(C)I	heptane	-4.41	-7.41	-7.67
1-iodo-2-methylpropane	CC(C)CI	heptane	-5.06	-8.65	-8.63
2-iodo-2-methylpropane	CC(C)(C)I	heptane	-4.64	-8.01	-7.84
diiodomethane	ICI	heptane	-5.92	-9.02	-9.49
1,2-diiodoethane	ICCI	heptane	-6.43	-10.13	-10.12
ethanol	CCO	heptane	-2.22	-4.45	-4.93
butan-1-ol	CCCCO	heptane	-3.64	-6.66	-7.21
2-butanol	CCC(C)O	heptane	-3.58	-6.38	-7.17
isobutanol	CC(C)CO	heptane	-3.65	-6.36	-7.24
2-methyl-isopropanol	CC(C)(C)O	heptane	-3.39	-5.40	-7.02
pentan-1-ol	CCCCCO	heptane	-4.39	-8.16	-8.42
3-methyl-1-butanol	CC(C)CCO	heptane	-4.34	-8.52	-8.31
2-pentanol	CCCC(C)O	heptane	-4.24	-8.58	-8.20
3-methyl-2-butanol	CC(C)(C)CO	heptane	-4.01	-7.63	-7.86
3,3-dimethyl-1-butanol	CC(C)(C)CCO	heptane	-4.73	-8.84	-9.22
2,3-dimethyl-2-butanol	CC(C)(C)(C)CO	heptane	-4.57	-7.95	-8.95
2-ethyl-1-butanol	CCC(CC)CO	heptane	-4.92	-9.89	-9.30
2-hexanol	CCCC(C)O	heptane	-4.97	-8.75	-9.40
2-methyl-1-pentanol	CCCC(C)CO	heptane	-4.94	-9.42	-9.30
2-methyl-2-pentanol	CCCC(C)(C)O	heptane	-4.71	-8.28	-9.15
4-methyl-2-pentanol	CC(C)CC(C)O	heptane	-4.79	-8.42	-9.17
1-octanol	CCCCCCCCO	heptane	-6.51	-11.37	-11.76
1-nonanol	CCCCCCCCCO	heptane	-7.30	-12.83	-13.02
1-decanol	CCCCCCCCCO	heptane	-7.90	-13.89	-14.08
1-undecanol	CCCCCCCCCCCO	heptane	-8.53	-14.78	-15.00
1-dodecanol	CCCCCCCCCCCCO	heptane	-9.18	-16.30	-16.09
cyclopentanol	OC1CCCC1	heptane	-4.77	-8.89	-8.85
cyclohexanol	OC1CCCCC1	heptane	-5.41	-8.96	-9.89
propylamine	CCCN	heptane	-3.01	-6.01	-6.12
butylamine	CCCCN	heptane	-3.74	-7.16	-7.34
sec-butylamine	CCC(C)N	heptane	-3.20	-6.67	-6.66
<i>tert</i> -butylamine	CC(C)(C)N	heptane	-3.02	-5.97	-6.53

pentylamine	CCCCCN	heptane	-4.48	-8.15	-8.57
hexylamine	CCCCCN	heptane	-5.04	-9.43	-9.56
heptylamine	CCCCCCN	heptane	-5.79	-10.75	-10.80
octylamine	CCCCCCCN	heptane	-6.45	-11.81	-11.84
nonylamine	CCCCCCCCN	heptane	-7.43	-12.93	-13.41
decylamine	CCCCCCCCCN	heptane	-7.77	-14.03	-14.12
dodecylamine	CCCCCCCCCCCN	heptane	-9.15		-16.35
tetradecylamine	CCCCCCCCCCCCCN	heptane	-10.46		-18.69
cyclopropylamine	NC1CC1	heptane	-3.73	-5.77	-6.80
cyclopentylamine	NC1CCCC1	heptane	-4.93	-8.17	-9.05
cyclohexylamine	NC1CCCCC1	heptane	-5.29	-9.13	-9.70
cycloheptylamine	NC1CCCCC1	heptane	-5.74	-10.01	-10.56
diethylamine	CCNCC	heptane	-3.79	-6.79	-7.79
dipropylamine	CCCNCCC	heptane	-5.02	-9.12	-9.81
triethylamine	CCN(CC)CC	heptane	-4.70	-8.23	-9.05
tributylamine	CCCN(CCCC)CCCC	heptane	-8.57	-14.95	-15.40
trimethylenimine	C1CNC1	heptane	-3.80	-6.53	-7.28
pyrrolidine	C1CCNC1	heptane	-4.40	-7.38	-8.29
hexamethylenimine	C1CCCNCC1	heptane	-5.61	-9.36	-10.42
3-methylphenol	Cc1cccc(O)c1	heptane	-5.73	-9.54	-10.25
benzene	c1ccccc1	heptane	-4.18	-7.30	-7.91
1,2,4-trimethylbenzene	Cc1ccc(C)c(C)c1	heptane	-5.98	-11.18	-10.58
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	heptane	-5.97	-11.05	-10.54
naphthalene	c1ccc2ccccc2c1	heptane	-6.91	-12.39	-12.03
biphenyl	c1ccc(cc1)c2ccccc2	heptane	-8.27	-14.24	-14.05
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	heptane	-6.24	-10.61	-10.85
1-bromo-4-chlorobenzene	Clc1ccc(Br)cc1	heptane	-6.75	-11.43	-11.75
1,4-dibromobenzene	BrC1ccc(Br)cc1	heptane	-7.14	-12.00	-12.34
trifluorotoluene	Cc1ccc(F)c(F)c1F	heptane	-4.49	-7.97	-8.48
nitrobenzene	[O-][N+](=O)c1ccccc1	heptane	-5.57	-10.69	-9.95
anisole	COc1ccccc1	heptane	-5.35	-9.85	-9.50
aniline	Nc1ccccc1	heptane	-5.65	-9.74	-9.97
acetonitrile	CC#N	heptane	-2.46	-4.20	-4.38
propionitrile	CCC#N	heptane	-3.26	-5.83	-5.69
valeronitrile	CCCC#N	heptane	-4.62	-8.16	-7.85
hexanenitrile	CCCCC#N	heptane	-5.39	-9.53	-9.10
octanenitrile	CCCCCCC#N	heptane	-6.80	-11.92	-11.39
nonanenitrile	CCCCCCCC#N	heptane	-7.48	-12.57	-12.58
decanenitrile	CCCCCCCCC#N	heptane	-8.37	-14.11	-13.91
undecanenitrile	CCCCCCCCCC#N	heptane	-8.56	-15.37	-14.27
dodecanenitrile	CCCCCCCCCCC#N	heptane	-9.63	-16.50	-15.82
tridecanenitrile	CCCCCCCCCCCC#N	heptane	-10.13	-17.50	-16.56
helium	[He]	heptane	1.85	1.85	1.72
neon	[Ne]	heptane	1.71	1.33	1.39
argon	[Ar]	heptane	0.54	-0.29	-0.30
krypton	[Kr]	heptane	-0.07	-1.32	-1.18
xenon	[Xe]	heptane	-0.93	-2.41	-2.52
carbon dioxide	O=C=O	heptane	0.09	-2.31	-1.11
tetrafluoromethane	FC(F)(F)F	heptane	0.50	-0.38	-0.67
sulfur dioxide	O=[S]=O	heptane	-2.09	-3.80	-4.38
sulfur hexafluoride	F[S](F)(F)(F)F	heptane	-0.27	-1.98	-1.78
difluorodichloromethane	FC(F)(Cl)Cl	heptane	-1.94	-4.52	-4.65
hexafluorobenzene	Fc1c(F)c(F)c(F)c(F)c1F	heptane	-3.06	-7.56	-7.37
chlorotrifluoromethane	FC(F)(F)Cl	heptane	-0.72	-3.07	-2.72
1-nitropropane	CCC[N+](=[O-])=O	heptane	-3.89	-9.03	-7.48
1-nitrobutane	CCCC[N+](=[O-])=O	heptane	-4.63	-10.38	-8.64
1-nitropentane	CCCCC[N+](=[O-])=O	heptane	-5.34	-11.06	-9.77
1-methylnaphthalene	Cc1cccc2ccccc12	heptane	-7.49	-12.92	-12.88
pyridine	c1ccncc1	heptane	-4.65	-7.59	-8.24
1,2,4-trichlorobenzene	Clc1ccc(Cl)c(Cl)c1	heptane	-7.06	-12.51	-12.03
2-chloro-2-methylpropane	CC(C)(C)Cl	heptane	-3.52	-6.33	-6.72
$\alpha$ -pinene	CC1=CCC2CC1C2(C)C	heptane	-6.66	-10.55	-11.36
$\beta$ -pinene	CC1(C)C2CCC(=C)C1C2	heptane	-6.63	-10.70	-11.31
water	O	heptane	-0.98	-2.29	-3.14
methane	C	octane	0.11	-0.97	-1.16
octane	CCCCCCCC	octane	-5.38	-9.92	-10.00
dodecane	CCCCCCCCCCCC	octane	-8.15	-14.73	-14.32
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	octane	-4.85	-8.39	-9.16
diethyl ether	CCOCC	octane	-3.33	-6.19	-6.68
dipropyl ether	CCCOCCC	octane	-4.62	-8.31	-8.66
dibutyl ether	CCCCOCCCC	octane	-5.94	-10.60	-10.70
n-butyl methyl ether	CCCCOC	octane	-4.07	-7.46	-7.84
methyl <i>tert</i> -butyl ether	COC(C)(C)C	octane	-3.51	-6.84	-6.91
ethyl <i>tert</i> -butyl ether	CCOC(C)(C)C	octane	-4.06	-7.69	-7.74
diisopropyl ether	CC(C)OC(C)C	octane	-4.28	-7.44	-8.10
tetrahydropyran	C1CCOCC1	octane	-4.46	-7.96	-8.40
1,4-dioxane	C1COCCO1	octane	-4.28	-7.41	-8.15
2-methyltetrahydrofuran	CC1CCCCO1	octane	-4.36	-7.51	-8.22
2,5,8-trioxanonane	COCOCOCOC	octane	-5.58	-9.75	-10.22
methanol	CO	octane	-1.33	-3.66	-3.57
ethanol	CCO	octane	-2.13	-4.66	-4.92
2-ethoxyethanol	CCOCCO	octane	-4.55	-8.97	-9.12
1-hexene	CCCCC=C	octane	-3.89	-7.26	-7.59

chlorotrifluoromethane	FC(F)(F)Cl	octane	-0.66	-2.25	-2.68
dichlorodifluoromethane	FC(F)(Cl)Cl	octane	-1.88	-4.08	-4.61
helium	[He]	octane	1.84	1.93	1.70
neon	[Ne]	octane	1.69	1.66	1.36
argon	[Ar]	octane	0.62	-0.09	-0.26
krypton	[Kr]	octane	0.01	-1.20	-1.19
xenon	[Xe]	octane	-0.83	-2.43	-2.51
oxygen	O=O	octane	0.72	0.03	-0.05
tetrafluoromethane	FC(F)(F)F	octane	0.56	-0.02	-0.62
sulfur hexafluoride	F[S](F)(F)(F)(F)F	octane	-0.18	-1.99	-1.70
carbon monoxide	C=O	octane	0.70	-0.27	-0.32
butyronitrile	CCCC#N	octane	-3.84	-7.23	-6.73
acetophenone	CC(=O)c1ccccc1	octane	-6.24	-10.68	-11.04
methyl propanoate	CCC(=O)OC	octane	-3.82	-7.01	-7.48
methyl decanoate	CCCCCCCCC(=O)OC	octane	-8.53	-14.37	-14.81
methyl undecanoate	CCCCCCCCC(=O)OC	octane	-9.01	-16.30	-15.58
methyl tridecanoate	CCCCCCCCC(=O)OC	octane	-10.04	-19.14	-17.41
propyl propanoate	CCCOC(=O)CC	octane	-5.03	-9.26	-9.40
pyridine	c1ccncc1	octane	-4.54	-7.53	-8.17
3-methylpyridine	Cc1ccncc1	octane	-5.25	-8.99	-9.29
4-methylpyridine	Cc1cncnc1	octane	-5.23	-9.01	-9.25
2-chlorobutane	CCC(C)Cl	octane	-3.85	-7.00	-7.46
1-chlorooctane	CCCCCCCCCl	octane	-6.66	-12.13	-11.80
2-chloro-2-methylpropane	CC(C)(C)Cl	octane	-3.52	-6.33	-6.89
methyl ethyl ketone	CCC(C)=O	octane	-3.53	-6.57	-6.95
2-pentanone	CCCC(C)=O	octane	-4.24	-7.70	-8.07
3-pentanone	CCC(=O)CC	octane	-4.28	-7.88	-8.16
1-butanenitrile	CCCC#N	octane	-3.84	-7.23	-6.73
3-methylpyridine	Cc1ccncc1	octane	-5.25	-8.99	-9.29
4-methylpyridine	Cc1cncnc1	octane	-5.23	-9.01	-9.25
1-chloronaphthalene	Clc1cccc2ccccc12	octane	-7.97	-14.72	-13.75
methylbenzoate	COC(=O)c1ccccc1	octane	-6.56	-11.68	-11.64
ethylbenzoate	CCOC(=O)c1ccccc1	octane	-7.16	-12.64	-12.57
triethylamine	CCN(CC)CC	octane	-4.56	-8.27	-8.96
tributylamine	CCCCN(CCCC)CCCC	octane	-8.43	-14.94	-15.32
phenylacetone	CC(=O)Cc1ccccc1	octane	-6.73	-10.66	-11.66
nonane	CCCCCCCCC	nonane	-6.06	-11.10	-11.15
cycloheptane	C1CCCCC1	nonane	-4.88	-9.01	-9.07
cyclooctane	C1CCCCC1	nonane	-5.58	-10.16	-10.16
bromobenzene	Brc1ccccc1	nonane	-5.67	-9.76	-10.44
neon	[Ne]	nonane	1.68	1.50	1.34
argon	[Ar]	nonane	0.68	-0.35	-0.22
xenon	[Xe]	nonane	-0.77	-2.38	-2.53
ethyl acetate	CCOC(C)=O	nonane	-3.62	-6.84	-7.22
methyl nonanoate	CCCCCCCCC(=O)OC	nonane	-7.60	-13.98	-13.49
methyl decanoate	CCCCCCCCC(=O)OC	nonane	-8.47	-15.16	-14.81
cyclopentanone	O=C1CCCC1	nonane	-4.50	-8.24	-8.41
cyclohexanone	O=C1CCCCC1	nonane	-5.21	-9.18	-9.52
cycloheptanone	O=C1CCCCC1	nonane	-5.92	-10.49	-10.65
ethane	CC	decane	-0.59	-1.86	-2.52
propane	CCC	decane	-1.39	-3.28	-3.80
butane	CCCC	decane	-2.18	-4.85	-5.04
hexane	CCCCCC	decane	-3.74	-7.53	-7.53
decane	CCCCCCCCC	decane	-6.78	-12.28	-12.38
dodecane	CCCCCCCCCCCC	decane	-8.14	-14.74	-14.55
2-methylpentane	CCCC(C)C	decane	-3.62	-7.11	-7.34
3-methylpentane	CCC(C)CC	decane	-3.61	-7.20	-7.31
2,3-dimethylbutane	CC(C)(C)C	decane	-3.52	-6.89	-7.17
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	decane	-4.61	-8.35	-8.93
diethyl ether	CCOCC	decane	-3.10	-6.13	-6.45
dipropyl ether	CCOCCC	decane	-4.57	-8.28	-8.78
dibutyl ether	CCCCOCCC	decane	-5.94	-10.58	-10.93
diisopropyl ether	CC(C)OC(C)C	decane	-4.24	-7.39	-8.27
n-butyl methyl ether	CCCCOC	decane	-3.88	-7.42	-7.70
ethyl tert-butyl ether	CCOC(C)(C)C	decane	-3.95	-7.70	-7.75
tetrahydrofuran	C1CCOC1	decane	-3.76	-6.87	-7.52
2,5,8,11-tetraoxadodecane	COCCOCCOCCOCC	decane	-7.28	-12.70	-13.01
2,5,8,11,14-pentaoxapentadecane	COCCOCCOCCOCCOCC	decane	-8.93	-13.52	-15.77
methyl decanoate	CCCCCCCCC(=O)OC	decane	-8.41	-15.23	-14.79
methyl methacrylate	COC(=O)C(C)=C	decane	-4.12	-7.93	-8.04
methanol	CO	decane	-1.04	-3.78	-3.24
1-nonanol	CCCCCCCCCO	decane	-7.21	-13.14	-13.27
1-undecanol	CCCCCCCCCCO	decane	-8.42	-15.27	-15.23
2-methyl-2-butanol	CCC(C)(C)O	decane	-3.79	-6.76	-8.03
helium	[He]	decane	1.82	1.64	1.66
neon	[Ne]	decane	1.67	1.56	1.32
argon	[Ar]	decane	0.69	-0.39	-0.21
krypton	[Kr]	decane	0.13	-1.16	-1.19
xenon	[Xe]	decane	-0.71	-2.35	-2.54
nitrogen	N#N	decane	1.09	-0.07	0.50
carbon monoxide	C=O	decane	0.78	0.09	-0.34
carbon dioxide	O=C=O	decane	0.16	-1.65	-1.47



oxygen	O=O	decane		0.68	-0.06	-0.24
acetophenone	CC(=O)c1ccccc1	decane		-6.12	-10.70	-11.01
3-methylpyridine	Cc1ccncc1	decane		-5.05	-8.95	-9.11
4-methylpyridine	Cc1ccncc1	decane		-5.04	-8.98	-9.07
methyl ethyl ketone	CCC(C)=O	decane		-3.42	-6.56	-6.95
3-pentanone	CCC(=O)CC	decane		-4.16	-7.85	-8.12
2-hexanone	CCCCC(C)=O	decane		-4.81	-8.70	-9.13
tetrachloromethane	ClC(Cl)(Cl)Cl	decane		-3.99	-7.45	-7.66
xenon	[Xe]	undecane		-0.68	-2.30	-2.55
methane	C	dodecane		0.23	-0.94	-0.97
propane	CCC	dodecane		-1.26	-3.65	-3.69
hexane	CCCCCC	dodecane		-3.61	-7.51	-7.42
heptane	CCCCCCC	dodecane		-4.39	-8.72	-8.66
octane	CCCCCCCC	dodecane		-5.09	-9.90	-9.80
decane	CCCCCCCCC	dodecane		-6.64	-12.28	-12.23
2,4-dimethylpentane	CC(C)CC(C)C	dodecane		-4.13	-7.72	-8.24
1-hexene	CCCCC=C	dodecane		-3.59	-7.21	-7.37
dibutyl ether	CCCCOCCCC	dodecane		-5.83	-10.54	-10.84
diisopropyl ether	CC(C)OC(C)C	dodecane		-4.07	-7.27	-8.03
n-butyl methyl ether	CCCCOC	dodecane		-3.71	-7.43	-7.47
ethyl tert-butyl ether	CCOC(C)(C)C	dodecane		-3.77	-7.65	-7.51
2-methyltetrahydrofuran	CC1CCCCO1	dodecane		-4.21	-7.47	-8.26
2,5,8,11-tetraoxadodecane	COCCOCCOCCOC	dodecane		-7.08	-12.81	-12.77
2-octanone	CCCCCCC(C)=O	dodecane		-6.01	-11.08	-11.01
2-decanone	CCCCCCCCC(C)=O	dodecane		-7.32	-13.29	-13.08
methyl decanoate	CCCCCCCCC(=O)OC	dodecane		-8.26	-15.15	-14.59
methyl methacrylate	COC(=O)C(C)=C	dodecane		-3.81	-7.84	-7.52
1,4-difluorobenzene	Fc1ccc(F)cc1	dodecane		-3.72	-7.76	-7.54
1-chloronaphthalene	Clc1cccc2ccccc12	dodecane		-7.99	-14.91	-14.13
helium	[He]	dodecane		1.79	1.72	1.62
neon	[Ne]	dodecane		1.66	1.67	1.29
argon	[Ar]	dodecane		0.71	-0.15	-0.19
butyronitrile	CCCC#N	dodecane		-3.48	-7.85	-6.30
pyridine	c1ccncc1	dodecane		-4.18	-7.61	-7.78
3-methylpyridine	Cc1ccncc1	dodecane		-4.90	-8.97	-8.90
4-methylpyridine	Cc1ccncc1	dodecane		-4.88	-8.97	-8.87
tridecane	CCCCCCCCCCCC	tridecane		-8.66	-15.89	-15.50
xenon	[Xe]	tridecane		-0.64	-2.28	-2.56
tetradecane	CCCCCCCCCCCCC	tetradecane		-9.39	-17.07	-16.58
diethyl ether	CCOCC	tetradecane		-2.82	-6.02	-5.98
diisopropyl ether	CC(C)OC(C)C	tetradecane		-3.95	-7.28	-7.79
methyl tert-butyl ether	COC(C)(C)C	tetradecane		-3.01	-6.34	-6.23
1-hexene	CCCCC=C	tetradecane		-3.54	-7.18	-7.26
benzene	c1ccccc1	tetradecane		-3.69	-7.31	-7.45
hexafluorobenzene	Fc1c(F)c(F)c(F)c(F)c1F	tetradecane		-2.90	-7.73	-7.10
3-pentanone	CCC(=O)CC	tetradecane		-3.71	-7.57	-7.30
2-decanone	CCCCCCCCC(C)=O	tetradecane		-7.27	-13.24	-12.95
helium	[He]	tetradecane		1.74	1.41	1.60
neon	[Ne]	tetradecane		1.66	1.41	1.30
argon	[Ar]	tetradecane		0.68	-0.35	-0.19
krypton	[Kr]	tetradecane		0.21	-1.27	-1.10
xenon	[Xe]	tetradecane		-0.65	-2.24	-2.56
methyl decanoate	CCCCCCCCC(=O)OC	tetradecane		-8.23	-15.13	-14.49
pentadecane	CCCCCCCCCCCCC	pentadecane		-9.96	-17.81	-17.41
1-chloronaphthalene	Clc1cccc2ccccc12	pentadecane		-7.96	-14.91	-14.05
xenon	[Xe]	pentadecane		-0.65	-2.23	-2.58
methane	C	hexadecane		0.10	-0.95	-0.95
ethane	CC	hexadecane		-0.67	-2.75	-2.43
propane	CCC	hexadecane		-1.34	-3.81	-3.69
butane	CCCC	hexadecane		-2.03	-4.97	-4.95
pentane	CCCCC	hexadecane		-2.81	-6.20	-6.18
hexane	CCCCCC	hexadecane		-3.56	-7.42	-7.37
octane	CCCCCCCC	hexadecane		-4.91	-9.83	-9.41
hexadecane	CCCCCCCCCCCCCCC	hexadecane		-10.44	-19.45	-18.01
isobutane	CC(C)C	hexadecane		-1.93	-4.48	-4.76
cyclohexane	C1CCCCC1	hexadecane		-4.10	-7.53	-8.20
ethene	C=C	hexadecane		-0.62	-2.67	-2.43
propene	CC=C	hexadecane		-1.23	-3.19	-3.54
acetone	CC(C)=O	hexadecane		-2.31	-5.12	-5.34
methyl ethyl ketone	CCC(C)=O	hexadecane		-3.08	-6.33	-6.52
2-pentanone	CCCC(C)=O	hexadecane		-3.79	-7.42	-7.62
2-hexanone	CCCCC(C)=O	hexadecane		-4.50	-8.55	-8.71
4-heptanone	CCCC(=O)CCC	hexadecane		-5.22	-10.73	-9.86
2-octanone	CCCCCCC(C)=O	hexadecane		-5.96	-10.73	-10.99
2-nonanone	CCCCCCCC(C)=O	hexadecane		-6.65	-11.80	-12.08
2-decanone	CCCCCCCCC(C)=O	hexadecane		-7.28	-13.21	-13.03
cyclohexanone	O=C1CCCCC1	hexadecane		-5.10	-8.72	-9.76
dibutyl ether	CCCCOCCCC	hexadecane		-5.74	-10.38	-10.69
butyl methyl ether	CCCCOC	hexadecane		-3.63	-7.30	-7.40
tetrahydrofuran	C1CCOC1	hexadecane		-3.71	-6.82	-7.78
2-methyltetrahydrofuran	CC1CCCO1	hexadecane		-4.29	-7.36	-8.65
chloroform	ClC(Cl)Cl	hexadecane		-3.46	-6.71	-6.76
tetrachloromethane	ClC(Cl)(Cl)Cl	hexadecane		-4.00	-7.39	-7.57

1-chlorobutane	CCCCCl	hexadecane	-3.69	-7.38	-7.57
tetrachloroethene	ClC(Cl)=C(Cl)Cl	hexadecane	-4.38	-9.18	-8.43
nitromethane	C[N+](=O)[O-]	hexadecane	-2.38	-6.06	-5.79
2-nitropropane	CC(C)[N+](=O)[O-]	hexadecane	-3.66	-7.21	-7.78
acetonitrile	CC#N	hexadecane	-2.23	-4.56	-4.51
methanol	CO	hexadecane	-1.15	-3.19	-3.53
1-propanol	CCCO	hexadecane	-2.57	-5.06	-6.11
isopropanol	CC(C)O	hexadecane	-2.37	-5.35	-5.78
1-butanol	CCCCO	hexadecane	-3.30	-6.71	-7.29
1-pentanol	CCCCCO	hexadecane	-3.97	-7.49	-8.31
1-hexanol	CCCCCCO	hexadecane	-4.89	-9.51	-9.82
1-octanol	CCCCCCCCO	hexadecane	-6.27	-11.73	-11.96
1-undecanol	CCCCCCCCCO	hexadecane	-8.37	-14.67	-15.38
tert-butanol	CC(C)(C)O	hexadecane	-2.99	-5.50	-6.98
cyclohexanol	OC1CCCCC1	hexadecane	-5.49	-11.36	-10.91
ethyl acetate	CCOC(C)=O	hexadecane	-3.12	-6.69	-6.54
butyl acetate	CCCCOC(C)=O	hexadecane	-4.49	-9.20	-8.66
methyl decanoate	CCCCCCCCC(=O)OC	hexadecane	-8.24	-15.17	-14.53
methyl benzoate	COC(=O)c1ccccc1	hexadecane	-6.11	-11.56	-11.13
benzene	c1ccccc1	hexadecane	-3.62	-7.26	-7.26
toluene	Cc1ccccc1	hexadecane	-4.32	-8.58	-8.35
ethylbenzene	CCc1ccccc1	hexadecane	-5.08	-9.59	-9.55
propylbenzene	CCCc1ccccc1	hexadecane	-5.83	-10.55	-10.71
m-xylene	Cc1ccc(C)c1	hexadecane	-5.01	-9.89	-9.44
p-xylene	Cc1cc(C)cc1	hexadecane	-5.02	-9.92	-9.45
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	hexadecane	-5.70	-11.13	-10.52
acetophenone	CC(=O)c1ccccc1	hexadecane	-5.95	-11.32	-10.86
benzaldehyde	O=Cc1ccccc1	hexadecane	-5.28	-9.84	-9.85
benzonitrile	N#Cc1ccccc1	hexadecane	-5.45	-9.86	-9.40
chlorobenzene	Clc1ccccc1	hexadecane	-4.98	-9.14	-9.47
1,4-difluorobenzene	Fc1ccc(F)cc1	hexadecane	-3.63	-7.69	-7.40
aniline	Nc1ccccc1	hexadecane	-5.08	-9.99	-9.55
nitrobenzene	[O-][N+](=O)c1ccccc1	hexadecane	-5.50	-10.91	-10.56
N,N-dimethylaniline	CN(C)c1ccccc1	hexadecane	-5.91	-11.56	-10.90
pyridine	c1ccncc1	hexadecane	-4.26	-7.80	-8.07
2-methylpyridine	Cc1cccn1	hexadecane	-4.96	-8.58	-9.22
3-methylpyridine	Cc1ccncc1	hexadecane	-5.03	-8.96	-9.33
4-methylpyridine	Cc1cncnc1	hexadecane	-5.00	-8.79	-9.25
propylamine	CCCN	hexadecane	-2.44	-5.73	-5.65
butylamine	CCCCN	hexadecane	-3.20	-7.03	-6.95
pentylamine	CCCCCN	hexadecane	-3.94	-8.32	-8.19
hexylamine	CCCCCCN	hexadecane	-4.61	-9.43	-9.44
nonylamine	CCCCCCCCCN	hexadecane	-6.90	-13.15	-13.08
diethylamine	CCNCC	hexadecane	-3.50	-5.88	-7.87
triethylamine	CCN(CC)CC	hexadecane	-4.19	-8.16	-8.62
neon	[Ne]	hexadecane	1.64	1.62	1.26
argon	[Ar]	hexadecane	0.62	-0.19	-0.25
krypton	[Kr]	hexadecane	0.17	-1.20	-1.05
xenon	[Xe]	hexadecane	-0.67	-2.41	-2.58
radon	[Rn]	hexadecane	-0.72	-3.39	-2.57
hydrogen	[H][H]	hexadecane	1.38	1.09	0.93
2,2,2-trifluoroethanol	OCC(F)(F)F	hexadecane	-2.00	-4.99	-5.64
1,1,1,3,3,3-hexafluoropropan-2-ol	OC(C(F)(F)F)C(F)(F)F	hexadecane	-1.93	-5.28	-5.48
benzyl alcohol	OCc1ccccc1	hexadecane	-5.83	-10.13	-11.22
thiophene	s1ccccc1	hexadecane	-3.91	-7.15	-7.35
benzyl chloride	ClCc1ccccc1	hexadecane	-5.82	-10.35	-10.72
1-chloronaphthalene	Clc1ccc2ccccc12	hexadecane	-8.02	-14.76	-14.19
1-methylnaphthalene	Cc1ccc2ccccc12	hexadecane	-7.32	-13.34	-13.02
methyl tert-amyl ether	CCC(C)(C)OC	hexadecane	-3.74	-8.15	-7.51
2,2-dimethylpropane	CC(C)(C)C	hexadecane	-2.25	-5.05	-5.28
methane	C	1-octanol	0.59	-0.93	-0.65
pentane	CCCCC	1-octanol	-2.40	-6.10	-5.58
hexane	CCCCCC	1-octanol	-3.19	-7.25	-6.87
heptane	CCCCCCC	1-octanol	-3.94	-8.44	-8.13
octane	CCCCCCCC	1-octanol	-4.59	-9.58	-9.22
nonane	CCCCCCCCC	1-octanol	-5.46	-10.73	-10.67
dodecane	CCCCCCCCCCC	1-octanol	-7.57	-14.13	-14.20
cyclohexane	C1CCCCC1	1-octanol	-3.77	-8.48	-7.53
cyclooctane	C1CCCCCCC1	1-octanol	-5.26	-9.94	-10.03
bicyclohexyl	C1CCC(CC1)C2CCCCC2	1-octanol	-8.05	-13.53	-13.95
methylcyclohexane	CC1CCCCC1	1-octanol	-4.43	-8.21	-8.68
ethene	C=C	1-octanol	-0.59	-1.49	-2.67
1-pentene	CCCC=C	1-octanol	-2.61	-5.35	-5.80
1-hexene	CCCCC=C	1-octanol	-3.38	-6.35	-7.05
1-heptene	CCCCC=C	1-octanol	-4.15	-8.26	-8.35
cyclohexene	C1CCC=CC1	1-octanol	-3.94	-9.12	-7.78
dichloromethane	ClCCl	1-octanol	-2.88	-6.66	-6.03
trichloromethane	ClC(Cl)Cl	1-octanol	-3.69	-7.81	-7.42
tetrachloromethane	ClC(Cl)(Cl)Cl	1-octanol	-3.83	-6.87	-7.76
1,1-dichloroethane	CC(Cl)Cl	1-octanol	-3.75	-6.85	-7.27
1,2-dichloroethane	ClCCCl	1-octanol	-3.96	-7.07	-7.58
1,1,2-trichloroethane	ClCC(Cl)Cl	1-octanol	-5.06	-8.78	-9.31

1,1,1,2-tetrachloroethane	<chem>ClCC(Cl)(Cl)Cl</chem>	1-octanol	-6.06	-10.10	-10.93
1,2-dichloropropane	<chem>CC(Cl)CCl</chem>	1-octanol	-4.72	-7.81	-8.69
1-chlorobutane	<chem>CCCCl</chem>	1-octanol	-3.63	-7.41	-7.26
2-chlorobutane	<chem>CCC(C)Cl</chem>	1-octanol	-3.49	-6.90	-7.02
1-chloropentane	<chem>CCCCCl</chem>	1-octanol	-4.28	-8.59	-8.28
1-chlorooctane	<chem>CCCCCCCCl</chem>	1-octanol	-6.42	-11.94	-11.84
dibromomethane	<chem>BrCBr</chem>	1-octanol	-4.21	-9.10	-8.49
trichloroethylene	<chem>ClC=C(Cl)Cl</chem>	1-octanol	-3.98	-8.23	-7.93
diethyl ether	<chem>CCOCC</chem>	1-octanol	-2.97	-5.94	-6.11
di-n-propyl ether	<chem>CCOCCC</chem>	1-octanol	-4.30	-7.93	-8.36
di-isopropyl ether	<chem>CC(C)OC(C)C</chem>	1-octanol	-3.60	-7.42	-7.13
dibutyl ether	<chem>CCCCOCCCC</chem>	1-octanol	-5.73	-10.18	-10.74
methyl <i>tert</i> -butyl ether	<chem>COC(C)(C)C</chem>	1-octanol	-2.78	-6.70	-5.77
tetrahydrofuran	<chem>C1CCOC1</chem>	1-octanol	-3.61	-6.77	-7.01
tetrahydropyran	<chem>C1CCOCC1</chem>	1-octanol	-4.28	-7.33	-8.09
1,4-dioxane	<chem>C1COCCO1</chem>	1-octanol	-4.47	-6.87	-8.48
propanone	<chem>CC(C)=O</chem>	1-octanol	-2.53	-5.35	-4.99
butanone	<chem>CCC(C)=O</chem>	1-octanol	-3.31	-6.54	-6.24
pentan-2-one	<chem>CCCC(C)=O</chem>	1-octanol	-4.11	-7.42	-7.62
pentan-3-one	<chem>CCC(=O)CC</chem>	1-octanol	-4.11	-7.85	-7.54
hexan-2-one	<chem>CCCCC(C)=O</chem>	1-octanol	-4.93	-8.63	-9.00
heptan-4-one	<chem>CCCC(=O)CCC</chem>	1-octanol	-5.67	-9.67	-10.27
octan-2-one	<chem>CCCCCCC(C)=O</chem>	1-octanol	-6.32	-10.97	-11.26
nonan-2-one	<chem>CC(CCCCCC)=O</chem>	1-octanol	-7.12	-12.02	-12.62
nonan-5-one	<chem>CCCCC(=O)CCCC</chem>	1-octanol	-6.93	-11.28	-12.42
cyclopentanone	<chem>O=C1CCCC1</chem>	1-octanol	-5.23	-8.21	-9.63
cyclohexanone	<chem>O=C1CCCCC1</chem>	1-octanol	-5.93	-8.91	-10.75
acetophenone	<chem>CC(=O)c1ccccc1</chem>	1-octanol	-6.66	-12.01	-11.23
ethyl acetate	<chem>CCOC(C)=O</chem>	1-octanol	-3.24	-6.64	-6.09
propyl acetate	<chem>CCOC(C)=O</chem>	1-octanol	-4.01	-7.89	-7.46
butyl acetate	<chem>CCCCOC(C)=O</chem>	1-octanol	-4.63	-8.87	-8.53
pentyl acetate	<chem>CCCCCOC(C)=O</chem>	1-octanol	-5.36	-9.87	-9.79
methyl formate	<chem>COC=O</chem>	1-octanol	-2.48	-5.11	-4.97
propyl formate	<chem>CCOC=O</chem>	1-octanol	-3.53	-7.26	-6.73
methyl propionate	<chem>CCC(=O)OC</chem>	1-octanol	-3.30	-6.37	-6.20
ethyl propionate	<chem>CCOC(=O)CC</chem>	1-octanol	-4.08	-7.78	-7.58
methyl butanoate	<chem>CCCC(=O)OC</chem>	1-octanol	-4.19	-7.90	-7.77
methyl pentanoate	<chem>CCCCC(=O)OC</chem>	1-octanol	-4.80	-8.85	-8.77
methyl benzoate	<chem>COC(=O)c1ccccc1</chem>	1-octanol	-6.95	-11.78	-11.84
ethyl benzoate	<chem>CCOC(=O)c1ccccc1</chem>	1-octanol	-7.61	-13.03	-13.02
propyl benzoate	<chem>CCOC(=O)c1ccccc1</chem>	1-octanol	-8.24	-14.03	-14.12
butyl benzoate	<chem>CCCCOC(=O)c1ccccc1</chem>	1-octanol	-9.09	-15.01	-15.58
methanol	<chem>CO</chem>	1-octanol	-3.33	-8.86	-8.35
ethanol	<chem>CCO</chem>	1-octanol	-3.97	-9.99	-9.48
propan-1-ol	<chem>CCCO</chem>	1-octanol	-4.76	-11.22	-10.81
butan-1-ol	<chem>CCCCO</chem>	1-octanol	-5.28	-12.39	-11.62
2-butanol	<chem>CCC(C)O</chem>	1-octanol	-4.90	-11.81	-10.91
2,2-dimethyl-1-propanol	<chem>CC(C)(C)CO</chem>	1-octanol	-4.84	-12.82	-10.86
hexan-1-ol	<chem>CCCCCCO</chem>	1-octanol	-6.63	-14.70	-13.87
octan-1-ol	<chem>CCCCCCCCO</chem>	1-octanol	-8.27	-16.96	-16.58
decan-1-ol	<chem>CCCCCCCCCO</chem>	1-octanol	-9.44	-19.46	-18.42
toluene	<chem>Cc1ccccc1</chem>	1-octanol	-4.39	-8.60	-8.25
ethylbenzene	<chem>CCc1ccccc1</chem>	1-octanol	-5.19	-9.54	-9.55
<i>o</i> -xylene	<chem>Cc1ccccc1C</chem>	1-octanol	-5.01	-9.93	-9.25
<i>m</i> -xylene	<chem>Cc1cccc(C)c1</chem>	1-octanol	-5.04	-9.80	-9.28
<i>p</i> -xylene	<chem>Cc1ccc(C)cc1</chem>	1-octanol	-5.04	-9.70	-9.28
1,3,5-trimethylbenzene	<chem>Cc1cc(C)cc(C)c1</chem>	1-octanol	-5.68	-10.97	-10.30
1,2-dichlorobenzene	<chem>Clc1ccccc1Cl</chem>	1-octanol	-6.22	-11.78	-11.15
1,2,3,4-tetrachlorobenzene	<chem>Clc1ccc(Cl)c(Cl)c1Cl</chem>	1-octanol	-8.30	-14.89	-14.70
1,2,4,5-tetrachlorobenzene	<chem>Clc1cc(Cl)c(Cl)cc1Cl</chem>	1-octanol	-8.54	-14.53	-14.91
aniline	<chem>Nc1ccccc1</chem>	1-octanol	-7.50	-12.23	-13.84
nitrobenzene	<chem>[O-][N+](=O)c1ccccc1</chem>	1-octanol	-6.47	-11.27	-11.14
benzonitrile	<chem>N#Cc1ccccc1</chem>	1-octanol	-7.02	-10.05	-10.94
phenanthrene	<chem>c1ccc2c(c1)ccc3ccccc23</chem>	1-octanol	-10.37	-18.04	-17.51
pyrene	<chem>c1cc2ccc3ccccc4ccc(c1)c2c34</chem>	1-octanol	-12.20	-18.24	-20.63
acetonitrile	<chem>CC#N</chem>	1-octanol	-3.30	-5.37	-5.32
propionitrile	<chem>CCC#N</chem>	1-octanol	-4.00	-6.30	-6.52
butyronitrile	<chem>CCCC#N</chem>	1-octanol	-4.79	-7.50	-8.00
propylamine	<chem>CCCN</chem>	1-octanol	-4.36	-9.78	-9.97
butylamine	<chem>CCCCN</chem>	1-octanol	-5.05	-10.78	-11.23
pentylamine	<chem>CCCCCN</chem>	1-octanol	-5.73	-11.96	-12.42
1-heptylamine	<chem>CCCCCCN</chem>	1-octanol	-6.67	-14.27	-14.13
dipropylamine	<chem>CCCNCCC</chem>	1-octanol	-5.52	-12.15	-12.36
dibutylamine	<chem>CCCCNCCC</chem>	1-octanol	-6.44	-14.36	-14.14
triethylamine	<chem>CCN(CC)CC</chem>	1-octanol	-4.47	-10.42	-9.89
piperidine	<chem>C1CCNCC1</chem>	1-octanol	-5.98	-11.71	-12.20
<i>N</i> -methylpiperidine	<chem>CN1CCCC1</chem>	1-octanol	-5.41	-10.33	-10.80
formamide	<chem>NC=O</chem>	1-octanol	-6.31	-13.26	-12.94
methylformamide	<chem>CNC=O</chem>	1-octanol	-5.75	-12.33	-11.36
dimethylformamide	<chem>CN(C)C=O</chem>	1-octanol	-4.94	-9.82	-9.69
helium	<chem>[He]</chem>	1-octanol	2.01	0.94	2.01
xenon	<chem>[Xe]</chem>	1-octanol	-0.39	-2.30	-2.31
nitrogen	<chem>N#N</chem>	1-octanol	1.08	0.60	0.06

carbon monoxide	C=O	1-octanol	0.97	0.05	-0.38
carbon dioxide	O=C=O	1-octanol	0.28	-2.18	-1.51
2,2',4,5'-tetrachlorobiphenyl	Clc1ccc(c(Cl)c1)c2cc(Cl)ccc2Cl	1-octanol	-12.09	-18.22	-18.95
2,2',5,6'-tetrachlorobiphenyl	Clc1ccc(Cl)c(c1)c2c(Cl)ccc2Cl	1-octanol	-12.14	-18.15	-19.23
2,3',4,4',5-pentachlorobiphenyl	Clc1ccc(cc1Cl)c2cc(Cl)c(Cl)cc2Cl	1-octanol	-12.99	-21.48	-20.50
3,3',4,4',5-pentachlorobiphenyl	Clc1ccc(cc1Cl)c2cc(Cl)c(Cl)c(Cl)c2	1-octanol	-13.19	-22.29	-21.19
2,2',3,4,4',5'-hexachlorobiphenyl	Clc1ccc(c(Cl)c1Cl)c2cc(Cl)c(Cl)cc2Cl	1-octanol	-13.72	-21.49	-21.87
2,2',3,3',4,4',6-heptachlorobiphenyl	Clc1ccc(c(Cl)c1Cl)c2c(Cl)cc(Cl)c(Cl)c2Cl	1-octanol	-14.41	-21.77	-23.16
2,2',3,4,4',5,6-heptachlorobiphenyl	Clc1ccc(c(Cl)c1)c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl	1-octanol	-14.39	-20.75	-23.13
1,4-dichloronaphthalene	Clc1ccc(Cl)c2ccccc12	1-octanol	-9.36	-14.86	-15.59
1,4,5-trichloronaphthalene	Clc1ccc2c(Cl)ccc(Cl)c12	1-octanol	-10.47	-17.83	-17.47
1,2,4,5-tetrachloronaphthalene	Clc1cc(Cl)c2c(Cl)cccc2c1Cl	1-octanol	-11.62	-19.51	-19.45
1,2,4,8-tetrachloronaphthalene	Clc1cc(Cl)c2cccc(Cl)c2c1Cl	1-octanol	-11.58	-19.25	-19.37
1,2,5,8-tetrachloronaphthalene	Clc1ccc2c(Cl)ccc(Cl)c2c1Cl	1-octanol	-11.57	-19.13	-19.36
1,2,4,5,7-pentachloronaphthalene	Clc1cc(Cl)c2c(Cl)cc(Cl)c(Cl)c2c1	1-octanol	-12.23	-20.15	-20.08
1,2,4,6,8-pentachloronaphthalene	Clc1cc(Cl)c2c(Cl)c(Cl)cc(Cl)c2c1	1-octanol	-12.19	-20.21	-20.01
1,2,3,4,6-pentachloronaphthalene	Clc1ccc2c(Cl)c(Cl)c(Cl)c(Cl)c2c1	1-octanol	-12.40	-21.18	-20.73
1,2,4,7,8-pentachloronaphthalene	Clc1ccc2c(Cl)cc(Cl)c(Cl)c2c1Cl	1-octanol	-12.34	-20.37	-20.63
1,2,3,5,8-pentachloronaphthalene	Clc1ccc(Cl)c2c(Cl)c(Cl)c(Cl)cc12	1-octanol	-12.34	-21.44	-20.61
1,2,4,5,8-pentachloronaphthalene	Clc1ccc(Cl)c2c(Cl)c(Cl)cc(Cl)c12	1-octanol	-12.35	-22.02	-20.67
1,2,3,5,7,8-hexachloronaphthalene	Clc1cc(Cl)c2cc(Cl)c(Cl)c(Cl)c2c1Cl	1-octanol	-12.90	-22.46	-21.44
1,2,3,4,5,6-hexachloronaphthalene	Clc1ccc2c(Cl)c(Cl)c(Cl)c(Cl)c2c1Cl	1-octanol	-12.88	-21.35	-21.67
1,2,3,4,5,8-hexachloronaphthalene	Clc1ccc(Cl)c2c(Cl)c(Cl)c(Cl)c(Cl)c12	1-octanol	-12.77	-23.06	-21.47
N-methylpyrrolidine	CN1CCCC1	1-octanol	-4.88	-9.64	-9.82
pyrrolidine	C1CCNC1	1-octanol	-5.44	-11.44	-11.22
water	O	1-octanol	-3.80	-9.75	-10.13
tetramethylstannane	C[Sn](C)(C)C	1-octanol	-3.62	-7.24	-7.03
pentane	CCCCC	acetonitrile	-2.22	-4.25	-4.73
hexane	CCCCCC	acetonitrile	-2.80	-5.13	-5.64
heptane	CCCCCCC	acetonitrile	-3.37	-5.85	-6.57
octane	CCCCCCCC	acetonitrile	-3.99	-6.74	-7.66
undecane	CCCCCCCCCCC	acetonitrile	-6.00	-9.25	-10.90
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	acetonitrile	-3.32	-6.22	-6.77
cyclohexane	C1CCCCC1	acetonitrile	-3.25	-5.56	-6.07
methanol	CO	acetonitrile	-3.70	-7.68	-8.40
ethanol	CCO	acetonitrile	-4.27	-8.23	-9.45
1-butanol	CCCCO	acetonitrile	-5.40	-9.99	-11.39
1-hexanol	CCCCCCO	acetonitrile	-6.77	-11.93	-13.54
1-heptanol	CCCCCCCCO	acetonitrile	-7.30	-11.73	-14.47
1-octanol	CCCCCCCCCO	acetonitrile	-7.89	-13.26	-15.33
isobutanol	CC(C)CO	acetonitrile	-5.33	-9.61	-11.23
2-methyl-isopropanol	CC(C)(C)O	acetonitrile	-4.56	-8.86	-10.04
2-methyl-2-butanol	CCC(C)(C)O	acetonitrile	-4.89	-9.59	-10.65
3-methyl-1-butanol	CC(C)CCO	acetonitrile	-5.84	-10.62	-11.99
toluene	Cc1ccccc1	acetonitrile	-4.76	-8.92	-8.55
p-xylene	Cc1ccc(C)cc1	acetonitrile	-5.21	-9.91	-9.23
aniline	Nc1ccccc1	acetonitrile	-7.30	-13.15	-12.82
nitromethane	C[N+](=O)[O-]	acetonitrile	-4.61	-9.17	-8.45
1-nitropropane	CCC[N+](=O)[O-]	acetonitrile	-5.77	-10.38	-10.20
acetonitrile	CC#N	acetonitrile	-4.44	-9.87	-7.00
butyronitrile	CCCC#N	acetonitrile	-5.69	-9.16	-9.13
hexanenitrile	CCCCCC#N	acetonitrile	-6.78	-10.82	-10.98
octanenitrile	CCCCCCCC#N	acetonitrile	-7.66	-12.38	-12.53
decanenitrile	CCCCCCCCC#N	acetonitrile	-8.90	-14.16	-14.51
1-chloropropane	CCCCl	acetonitrile	-3.24	-6.22	-6.23
1-chlorobutane	CCCCCl	acetonitrile	-3.90	-7.17	-7.28
chloroform	ClC(Cl)Cl	acetonitrile	-4.17	-7.78	-7.85
tetrachloromethane	ClC(Cl)(Cl)Cl	acetonitrile	-4.17	-7.03	-7.91
cis-1,2-dichloroethene	ClC=C/Cl	acetonitrile	-3.69	-7.59	-7.06
trans-1,2-dichloroethene	ClC=C\Cl	acetonitrile	-4.01	-7.06	-7.39
trichloroethene	ClC=C(Cl)Cl	acetonitrile	-4.45	-7.88	-8.32
tetrachloroethene	ClC(Cl)=C(Cl)Cl	acetonitrile	-4.38	-8.32	-8.29
2-chloro-2-methylpropane	CC(C)(C)Cl	acetonitrile	-3.25	-6.20	-6.09
2-bromo-2-methylpropane	CC(C)(C)Br	acetonitrile	-3.45	-6.69	-6.52
1,1,2,2-tetrachloroethane	ClC(Cl)(Cl)Cl	acetonitrile	-6.88	-11.82	-11.99
2-octanone	CCCCCCC(C)=O	acetonitrile	-6.46	-11.40	-11.13
cyclohexanone	O=C1CCCCC1	acetonitrile	-5.94	-10.47	-10.24
benzophenone	O=C(c1ccccc1)c2ccccc2	acetonitrile	-11.12	-17.01	-17.68
diethylamine	CCNCC	acetonitrile	-4.36	-7.11	-9.88
sec-butylamine	CCC(C)N	acetonitrile	-3.92	-7.49	-9.33
triethylamine	CCN(CC)CC	acetonitrile	-4.02	-7.05	-8.63
dibutyl ether	CCCCOCCCC	acetonitrile	-5.44	-6.69	-9.74

pentyl propyl ether	CCCCOCCC	acetonitrile	-5.42		-9.71
isopropyl pentyl ether	CCCCOC(C)C	acetonitrile	-5.31		-9.66
methyl <i>tert</i> -butyl ether	COC(C)(C)C	acetonitrile	-3.46	-6.85	-6.67
2,5-dioxahexane	COCCOC	acetonitrile	-4.69	-9.27	-8.29
2,5,8-trioxanonane	COCCOCCOC	acetonitrile	-7.45	-12.31	-13.60
2,5,8,11-tetraoxadodecane	COCCOCCOCCOC	acetonitrile	-9.25	-16.73	-16.44
2,5,8,11,14-pentaoxapentadecane	COCCOCCOCCOCCOC	acetonitrile	-10.96	-20.67	-19.44
15-crown-5	C1COCCOCCOCCOCCO1	acetonitrile	-10.57	-19.88	-20.28
12-crown-4	C1COCCOCCOCCO1	acetonitrile	-8.79	-16.57	-16.64
methyl acetate	COC(C)=O	acetonitrile	-4.19	-7.85	-7.34
ethyl benzoate	CCOC(=O)c1ccccc1	acetonitrile	-7.97	-13.55	-13.17
propyl benzoate	CCCOC(=O)c1ccccc1	acetonitrile	-8.61	-14.34	-14.34
phenol	Oc1ccccc1	acetonitrile	-7.63	-14.20	-14.30
hydrogen	[H][H]	acetonitrile	1.62	1.56	1.20
2-chlorophenol	Oc1ccccc1Cl	acetonitrile	-8.07	-13.55	-14.55
3-chlorophenol	Oc1cccc(Cl)c1	acetonitrile	-8.90	-15.74	-16.17
3-methoxyphenol	COc1cccc(O)c1	acetonitrile	-9.54	-18.64	-17.51
biphenyl	c1ccc(cc1)[N+](=O)c2ccccc2	acetonitrile	-8.62	-14.39	-14.20
anthracene	c1ccc2cc3ccccc3cc2c1	acetonitrile	-10.29	-17.61	-16.94
sulfur dioxide	O=[S]=O	acetonitrile	-2.69	-7.10	-6.40
1-naphthol	Oc1cccc2ccccc12	acetonitrile	-10.81	-18.55	-19.27
carbon dioxide	O=C=O	acetonitrile	-0.97	-3.32	-3.29
diphenyl ether	O(c1ccccc1)c2ccccc2	acetonitrile	-9.56	-14.34	-15.40
2-nitrotoluene	Cc1ccccc1[N+](=O)[O-]	acetonitrile	-8.30	-13.41	-13.87
4-nitrotoluene	Cc1ccc(cc1)[N+](=O)[O-]	acetonitrile	-8.08	-13.36	-13.56
dimethyl phthalate	COC(=O)c1ccccc1C(=O)OC	acetonitrile	-9.69	-18.04	-15.60
1,3-dichlorobenzene	Clc1cccc(Cl)c1	acetonitrile	-6.56	-10.37	-11.04
1,2-dibromobenzene	Brcc1ccccc1Br	acetonitrile	-7.02	-11.78	-11.81
1,3-dibromobenzene	Brcc1cccc(Br)c1	acetonitrile	-7.26	-11.82	-12.12
1,2-diiodobenzene	Ic1ccccc1I	acetonitrile	-8.86	-13.90	-13.85
1,3-diiodobenzene	Ic1cccc(I)c1	acetonitrile	-9.10	-13.83	-14.22
3-bromotoluene	Cc1cccc(Br)c1	acetonitrile	-5.99	-10.30	-10.11
4-bromotoluene	Cc1ccc(Br)cc1	acetonitrile	-5.99	-10.02	-10.12
2-iodotoluene	Cc1ccccc1I	acetonitrile	-7.01	-11.01	-11.32
3-iodotoluene	Cc1cccc(I)c1	acetonitrile	-6.94	-11.11	-11.23
1-chloro-2-nitrobenzene	[O-][N+](=O)c1ccccc1Cl	acetonitrile	-7.70	-14.32	-12.93
1-chloro-3-nitrobenzene	[O-][N+](=O)c1cccc(Cl)c1	acetonitrile	-8.71	-13.72	-14.61
1-bromo-4-nitrobenzene	[O-][N+](=O)c1ccc(Br)cc1	acetonitrile	-8.89	-14.89	-14.83
dimethyl terephthalate	COC(=O)c1ccc(cc1)C(=O)OC	acetonitrile	-10.37	-17.83	-16.62
9-nitroanthracene	[O-][N+](=O)c1c2ccccc2cc3ccccc13	acetonitrile	-13.38	-22.23	-21.53
2,4,6-trinitrotoluene	Cc1c(cc(cc1[N+](=O)[O-])=O)[N+](=O)[O-]	acetonitrile	-13.10	-23.71	-22.08
3-methoxybenzamide	COc1cccc(c1)C(N)=O	acetonitrile	-12.71	-21.89	-22.64
formamide	NC=O	acetonitrile	-7.29	-13.19	-14.36
methylformamide	CNC=O	acetonitrile	-6.80	-11.88	-12.98
dimethylformamide	CN(C)C=O	acetonitrile	-5.74	-11.52	-10.84
<i>N</i> -methylacetamide	CNC(C)=O	acetonitrile	-7.39	-15.27	-14.40
<i>N,N</i> -dimethylacetamide	CN(C)C(C)=O	acetonitrile	-6.23	-12.60	-11.93
2-pyrrolidone	O=C1CCCN1	acetonitrile	-8.51	-15.22	-15.58
3-nitrophenol	Oc1cccc(c1)[N+](=O)[O-]	acetonitrile	-10.89	-19.79	-19.81
2,4,6-trimethylphenol	Cc1cc(C)c(C)c(C)c1	acetonitrile	-9.16	-15.65	-16.95
pyrrole	[nH]1ccccc1	acetonitrile	-5.85	-11.23	-10.59
nitrobenzene	[O-][N+](=O)c1ccccc1	acetonitrile	-7.48	-12.12	-12.59
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	acetonitrile	-7.47	-12.07	-12.03
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	acetonitrile	-9.44	-14.21	-16.59
1,2-dicyanobenzene	N#Cc1ccccc1C#N	acetonitrile	-10.47	-16.79	-15.51
1,4-dicyanobenzene	N#Cc1ccc(cc1)C#N	acetonitrile	-10.63	-16.01	-15.30
2-cyanonaphthalene	N#Cc1ccc2ccccc2c1	acetonitrile	-11.16	-15.83	-17.31
2-methylimidazole	Cc1[nH]ccn1	acetonitrile	-9.17	-15.44	-16.35
2-ethylimidazole	CCc1[nH]ccn1	acetonitrile	-9.69	-15.30	-17.14
2-isopropylimidazole	CC(C)c1[nH]ccn1	acetonitrile	-10.17	-16.44	-18.04
pyrazole	[nH]1cccn1	acetonitrile	-7.42	-13.38	-13.58
3,5-dimethylpyrazole	Cc1[nH]nc(C)c1	acetonitrile	-8.44	-14.56	-15.62
3,4,5-trimethylpyrazole	Cc1[nH]nc(C)c1C	acetonitrile	-8.92	-17.28	-16.56
$\gamma$ -butyrolactam	O=C1CCCN1	acetonitrile	-8.51	-16.32	-15.58
<i>N</i> -methylbutyrolactam	CN1CCCC1=O	acetonitrile	-7.41	-13.89	-13.34
$\delta$ -valerolactam	O=C1CCCCN1	acetonitrile	-8.89	-15.46	-16.31
<i>N</i> -methylvalerolactam	CN1CCCCC1=O	acetonitrile	-7.92	-14.13	-14.37
$\epsilon$ -caprolactam	O=C1CCCCCN1	acetonitrile	-9.38	-16.13	-17.39
<i>N</i> -methylcaprolactam	CN1CCCCC1=O	acetonitrile	-8.39	-14.96	-15.32
4-(dimethylamino)pyridine	CN(C)c1ccncc1	acetonitrile	-8.28	-15.11	-14.06
3-hydroxypyridine	Oc1ccncc1	acetonitrile	-9.71	-15.27	-17.54
3-aminopyridine	Nc1ccncc1	acetonitrile	-10.21	-15.13	-18.10
3-cyanopyridine	N#Cc1ccncc1	acetonitrile	-9.06	-13.13	-13.61
methyl nicotinate	COC(=O)c1ccncc1	acetonitrile	-8.82	-14.04	-14.22
water	O	acetonitrile	-4.13	-8.63	-10.12
tetramethylstannane	C[Sn](C)(C)C	acetonitrile	-3.50	-5.49	-6.15
<i>N</i> -methylimidazole	Cn1ccncc1	acetonitrile	-6.62	-0.33	-10.91
ethane	CC	acetone	-0.77	-2.06	-2.27
propane	CCC	acetone	-1.47	-3.84	-3.37
pentane	CCCCC	acetone	-2.60	-4.68	-5.08

heptane	CCCCCCC	acetone	-3.87	-6.40	-6.99
octane	CCCCCCCC	acetone	-4.58	-7.59	-8.23
nonane	CCCCCCCCC	acetone	-5.16	-8.53	-9.03
dodecane	CCCCCCCCCCCC	acetone	-7.10	-11.53	-12.18
hexadecane	CCCCCCCCCCCCCCC	acetone	-9.45	-15.15	-15.79
cyclohexane	C1CCCCC1	acetone	-3.50	-6.25	-5.98
adamantane	C1C2CC3CC1CC(C2)C3	acetone	-6.30	-9.66	-9.31
benzene	c1ccccc1	acetone	-4.29	-7.49	-7.52
toluene	Cc1ccccc1	acetone	-4.87	-8.84	-8.45
ethylbenzene	CCc1ccccc1	acetone	-5.52	-9.78	-9.43
<i>p</i> -xylene	Cc1ccc(C)cc1	acetone	-5.48	-10.04	-9.44
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	acetone	-6.06	-10.60	-10.37
1,2,4-trimethylbenzene	Cc1ccc(C)c(C)c1	acetone	-6.05	-11.01	-10.35
naphthalene	c1ccc2ccccc2c1	acetone	-7.54	-12.91	-12.65
biphenyl	c1ccc(cc1)c2ccccc2	acetone	-9.11	-14.89	-14.92
anthracene	c1ccc2cc3ccccc3cc2c1	acetone	-10.86	-18.19	-17.90
methanol	CO	acetone	-4.04	-8.10	-8.79
ethanol	CCO	acetone	-4.52	-9.00	-9.57
butan-1-ol	CCCCO	acetone	-5.58	-10.50	-11.11
2-butanol	CCC(C)O	acetone	-5.32	-10.20	-10.67
3-methyl-1-butanol	CC(C)CCO	acetone	-6.19	-11.55	-12.03
ethylene glycol	OCCO	acetone	-6.06	-12.79	-13.43
glycerol	OCC(O)CO	acetone	-6.41	-18.02	-14.83
argon	[Ar]	acetone	0.70	0.46	0.01
radon	[Rn]	acetone	-1.07	-2.51	-2.47
oxygen	O=O	acetone	1.09	0.03	0.55
nitrogen	N#N	acetone	0.95	0.42	0.79
2-bromo-2-methylpropane	CC(C)(C)Br	acetone	-3.79	-7.07	-6.96
<i>trans</i> -1,2-dichloroethene	ClC=C(Cl)Cl	acetone	-4.24	-7.77	-7.62
trichloroethene	ClC=C(Cl)Cl	acetone	-4.66	-8.47	-8.30
tetrachloroethene	ClC(Cl)=C(Cl)Cl	acetone	-4.70	-8.91	-8.44
1-chlorobutane	CCCCCl	acetone	-4.10	-7.55	-7.45
2-chloro-2-methylpropane	CC(C)(C)Cl	acetone	-3.54	-6.47	-6.51
tetrachloromethane	ClC(Cl)(Cl)Cl	acetone	-4.49	-7.64	-8.04
<i>N,N</i> -dimethylaniline	CN(C)c1ccccc1	acetone	-7.34	-12.34	-12.60
aniline	Nc1ccccc1	acetone	-7.81	-13.92	-13.73
bromobenzene	Brc1ccccc1	acetone	-5.83	-10.40	-9.86
benzaldehyde	O=Cc1ccccc1	acetone	-6.88	-11.75	-11.39
nitrobenzene	[O-][N+](=O)c1ccccc1	acetone	-7.73	-13.11	-13.26
1,4-dibromobenzene	Brc1ccc(Br)cc1	acetone	-7.56	-12.83	-12.62
4-nitrotoluene	Cc1ccc(cc1)[N+](=O)[O-]	acetone	-8.36	-14.90	-14.28
1,4-dinitrobenzene	[O-][N+](=O)c1ccc(cc1)[N+](=O)[O-]	acetone	-10.39	-17.64	-17.95
4-nitroaniline	Nc1ccc(cc1)[N+](=O)[O-]	acetone	-11.44	-22.26	-20.73
2-pentanone	CCCC(C)=O	acetone	-4.89	-9.05	-8.50
2-hexanone	CCCCC(C)=O	acetone	-5.51	-9.93	-9.44
2-octanone	CCCCCCC(C)=O	acetone	-6.85	-11.66	-11.54
phenol	Oc1ccccc1	acetone	-8.30	-15.80	-15.63
diethyl ether	CCOCC	acetone	-3.47	-6.24	-6.16
2,5,8-trioxanonane	COCCOCCOC	acetone	-7.01	-11.54	-12.03
1,4-dioxane	C1COCCO1	acetone	-4.81	-9.13	-8.02
1,3-dioxane	C1COCOC1	acetone	-4.27	-9.30	-7.07
12-crown-4	C1COCCOCCOCCO1	acetone	-8.50	-15.54	-15.31
15-crown-5	C1COCCOCCOCCOCCO1	acetone	-10.34	-18.70	-19.10
methyl benzoate	COC(=O)c1ccccc1	acetone	-7.91	-13.03	-13.06
ethyl benzoate	CCOC(=O)c1ccccc1	acetone	-8.42	-13.93	-13.86
propyl benzoate	CCCOC(=O)c1ccccc1	acetone	-8.88	-14.87	-14.52
butyl benzoate	CCCCOC(=O)c1ccccc1	acetone	-9.61	-15.70	-15.72
nitromethane	C[N+](=O)[O-]	acetone	-4.77	-9.33	-8.94
1-bromoadamantane	BrC12CC3CC(C(C3)C1)C2	acetone	-7.82	-12.81	-12.30
tetraethyltin	CC[Sn](CC)(CC)CC	acetone	-5.74	-9.68	-9.19
adipic acid	OC(=O)CCCC(O)=O	acetone	-12.93	-25.29	-25.51
dimethyl carbonate	COC(=O)OC	acetone	-4.77	-8.90	-8.01
diethyl carbonate	CCOC(=O)OCC	acetone	-5.11	-10.32	-8.38
acetonitrile	CC#N	acetone	-5.00	-8.01	-8.16
formamide	NC=O	acetone	-7.32	-14.15	-14.55
dimethylformamide	CN(C)C=O	acetone	-5.90	-11.40	-10.78
acetamide	CC(N)=O	acetone	-7.62	-14.68	-14.88
<i>N</i> -methylacetamide	CNC(C)=O	acetone	-7.41	-15.56	-14.09
<i>N,N</i> -dimethylacetamide	CC(N(C)C)=O	acetone	-6.35	-12.25	-11.54
2-pyrrolidone	O=C1CCCN1	acetone	-8.63	-15.63	-15.74
pyrrole	[nH]1ccccc1	acetone	-6.38	-12.12	-11.42
water	O	acetone	-4.22	-9.48	-9.87
$\gamma$ -butyrolactam	O=C1CCCN1	acetone	-8.63	-16.73	-15.74
$\delta$ -valerolactam	O=C1CCCCN1	acetone	-8.77	-15.49	-15.74
<i>N</i> -methylvalerolactam	CN1CCCCC1=O	acetone	-7.55	-13.96	-12.95
$\epsilon$ -caprolactam	O=C1CCCCCN1	acetone	-8.99	-16.23	-15.99
<i>N</i> -methylcaprolactam	CN1CCCCC1=O	acetone	-7.95	-14.82	-13.62
<i>N</i> -methylimidazole	Cn1ccnc1	acetone	-7.24	-12.83	-12.07
methane	C	cyclohexane	0.07	-0.72	-0.79
propane	CCC	cyclohexane	-1.63	-3.94	-3.49
pentane	CCCCC	cyclohexane	-3.16	-6.10	-5.89
hexane	CCCCCC	cyclohexane	-3.86	-7.27	-6.97

heptane	CCCCCCC	cyclohexane	-4.58	-8.35	-8.11
octane	CCCCCCCC	cyclohexane	-5.34	-9.48	-9.37
decane	CCCCCCCCC	cyclohexane	-6.71	-11.73	-11.44
dodecane	CCCCCCCCCCCC	cyclohexane	-8.14	-13.96	-13.78
tetradecane	CCCCCCCCCCCCC	cyclohexane	-9.53	-16.30	-15.97
2-methylbutane	CCC(C)C	cyclohexane	-3.04	-5.88	-5.69
3-ethylpentane	CCC(CC)CC	cyclohexane	-4.42	-8.19	-7.86
2,2-dimethylbutane	CCC(C)(C)C	cyclohexane	-3.62	-6.49	-6.75
2-methylpentane	CCCC(C)C	cyclohexane	-3.74	-6.91	-6.78
3-methylpentane	CCC(C)CC	cyclohexane	-3.74	-6.90	-6.78
2,2-dimethylpentane	CCCC(C)(C)C	cyclohexane	-4.32	-7.50	-7.84
2,3-dimethylbutane	CC(C)(C)C	cyclohexane	-3.66	-6.49	-6.66
2,4-dimethylpentane	CC(C)CC(C)C	cyclohexane	-4.33	-7.59	-7.70
3,3-diethylpentane	CCC(CC)(CC)CC	cyclohexane	-5.74	-9.98	-10.17
3-methylheptane	CCCCC(C)CC	cyclohexane	-5.16	-9.00	-9.02
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	cyclohexane	-4.91	-8.20	-8.79
2,2-dimethylhexane	CCCCC(C)(C)C	cyclohexane	-4.99	-8.50	-8.90
2,2,4,4-tetramethylpentane	CC(C)(C)CC(C)(C)C	cyclohexane	-5.16	-9.14	-9.14
2,2,5,5-tetramethylhexane	CC(C)(C)CCC(C)(C)C	cyclohexane	-5.88	-9.60	-10.25
cyclopentane	C1CCCC1	cyclohexane	-3.44	-6.82	-6.09
cyclohexane	C1CCCCC1	cyclohexane	-4.18	-7.90	-7.28
cycloheptane	C1CCCCC1	cyclohexane	-4.89	-9.20	-8.40
methylcyclohexane	CC1CCCC1	cyclohexane	-4.78	-8.46	-8.21
cis-1,2-dimethylcyclohexane	C[C@H]1CCCC[C@@H]1C	cyclohexane	-5.35	-9.09	-9.07
adamantane	C1C2CC3CC1CC(C2)C3	cyclohexane	-7.09	-11.78	-10.84
ethene	C=C	cyclohexane	-0.83	-2.16	-2.20
1-pentene	CCCC=C	cyclohexane	-3.17	-5.81	-5.91
1-hexene	CCCCC=C	cyclohexane	-3.90	-7.02	-7.05
1-heptene	CCCCC=C	cyclohexane	-4.59	-8.17	-8.13
1-octene	CCCCC=C	cyclohexane	-5.32	-9.31	-9.28
1-nonene	CCCCC=C	cyclohexane	-6.02	-10.45	-10.39
1-decene	CCCCC=C	cyclohexane	-6.73	-11.57	-11.51
1-tridecene	CCCCCCCCC=C	cyclohexane	-8.89	-15.15	-14.98
1-tetradecene	CCCCCCCCC=C	cyclohexane	-9.56	-16.27	-15.99
1-pentadecene	CCCCCCCCC=C	cyclohexane	-10.26	-17.44	-17.17
cis-2-octene	CCCC/C=C/C	cyclohexane	-5.40	-9.12	-9.45
trans-2-octene	CCCC/C=C/C	cyclohexane	-5.36	-9.14	-9.36
cis-4-octene	CCC/C=C/CCC	cyclohexane	-5.36	-9.08	-9.37
trans-4-octene	CCC/C=C/CCC	cyclohexane	-5.37	-9.01	-9.35
cyclopentene	C1CC=CC1	cyclohexane	-3.48	-6.50	-6.27
cyclohexene	C1CCC=CC1	cyclohexane	-4.15	-7.90	-7.26
1-methylcyclohexene	CC1=CCCCC1	cyclohexane	-4.75	-9.07	-8.16
cycloheptene	C1CCC=CCC1	cyclohexane	-4.85	-8.72	-8.34
cyclooctene	C1CCCC=CC1	cyclohexane	-5.18	-9.94	-8.70
1,3-cyclopentadiene	C1C=CC=C1	cyclohexane	-3.53	-6.32	-6.45
1,4-cyclohexadiene	C1C=CCC=C1	cyclohexane	-4.18	-7.76	-7.38
1,5-cyclooctadiene	C1CC=CCCC=C1	cyclohexane	-5.62	-10.16	-9.59
1,3,5-cycloheptatriene	C1C=CC=CC=C1	cyclohexane	-5.00	-8.84	-8.79
cyclooctatetraene	C1=CC=CC=CC1	cyclohexane	-5.68	-9.72	-9.90
norbornadiene	C1C2C=CC1C=C2	cyclohexane	-4.88	-8.02	-8.23
1-octyne	CCCCC#C	cyclohexane	-5.34	-9.22	-9.30
2-octyne	CCCCC#CC	cyclohexane	-5.37	-9.94	-9.36
dichloromethane	ClCCl	cyclohexane	-2.98	-6.03	-5.47
trichloromethane	ClC(Cl)Cl	cyclohexane	-3.73	-6.75	-6.59
tetrachloromethane	ClC(Cl)(Cl)Cl	cyclohexane	-4.38	-7.60	-7.66
1-chloropropane	CCCCl	cyclohexane	-3.26	-6.08	-6.01
1-chlorobutane	CCCCCl	cyclohexane	-3.96	-7.32	-7.11
2-chloro-2-methylpropane	CC(C)(C)Cl	cyclohexane	-3.73	-6.39	-6.77
trichloroethene	ClC=C(Cl)Cl	cyclohexane	-4.24	-7.70	-7.50
difluorodichloromethane	FC(F)(Cl)Cl	cyclohexane	-1.82	-4.72	-4.16
iodomethane	CI	cyclohexane	-3.40	-5.80	-5.92
diiodomethane	CI	cyclohexane	-6.29	-9.22	-9.85
1-iodopropane	CCCI	cyclohexane	-4.65	-7.88	-7.80
propionaldehyde	CCC=O	cyclohexane	-3.04	-5.11	-5.69
acetone	CC(C)=O	cyclohexane	-2.92	-5.04	-5.47
methyl ethyl ketone	CCC(C)=O	cyclohexane	-3.77	-6.38	-6.86
2-pentanone	CCCC(C)=O	cyclohexane	-4.47	-7.48	-7.98
2-heptanone	CCCCC(C)=O	cyclohexane	-5.86	-9.72	-10.15
4-heptanone	CCCC(=O)CCC	cyclohexane	-5.93	-9.47	-10.33
2-octanone	CCCCCCC(C)=O	cyclohexane	-6.59	-10.76	-11.30
2-nonanone	CCCCCCC(C)=O	cyclohexane	-7.27	-11.95	-12.39
5-nonanone	CCCCC(=O)CCCC	cyclohexane	-7.20	-11.68	-12.30
2-decanone	CCCCCCCC(C)=O	cyclohexane	-7.89	-12.55	-13.37
2-undecanone	CCCCCCCCC(C)=O	cyclohexane	-8.57	-13.60	-14.38
6-undecanone	CCCCC(=O)CCCCC	cyclohexane	-8.46	-13.45	-14.34
tert-butyl methyl ketone	CC(=O)C(C)(C)C	cyclohexane	-4.56	-7.42	-8.05
di-tert-butyl ketone	CC(C)(C)C(=O)C(C)(C)C	cyclohexane	-5.85	-9.81	-10.09
cyclopentanone	O=C1CCCC1	cyclohexane	-4.87	-8.04	-8.55
cyclohexanone	O=C1CCCCC1	cyclohexane	-5.53	-9.00	-9.53
cycloheptanone	O=C1CCCCC1	cyclohexane	-6.20	-10.14	-10.55
2,4-pentanedione	CC(=O)CC(=O)C	cyclohexane	-5.66	-7.97	-10.08
diethyl ether	CCOCC	cyclohexane	-3.40	-5.51	-6.28
diisopropyl ether	CC(C)OC(C)C	cyclohexane	-4.34	-7.25	-7.69

methyl <i>tert</i> -butyl ether	COC(C)(C)C	cyclohexane	-3.61	-6.80	-6.59
ethyl <i>tert</i> -butyl ether	CCOC(C)(C)C	cyclohexane	-4.18	-7.68	-7.46
tetrahydrofuran	C1CCOC1	cyclohexane	-4.16	-6.86	-7.63
butyl methyl ether	CCCCOC	cyclohexane	-4.13	-7.09	-7.46
dimethoxymethane	COCOC	cyclohexane	-3.37	-5.67	-6.26
1,2-dimethoxyethane	COCCOC	cyclohexane	-4.14	-7.05	-7.40
1,3-dioxane	C1COCOC1	cyclohexane	-4.41	-7.47	-7.94
1,4-dioxane	C1COCCO1	cyclohexane	-4.56	-7.40	-8.18
2-methyltetrahydrofuran	CC1CCCO1	cyclohexane	-4.69	-7.60	-8.42
2,5-dimethyltetrahydrofuran	CC1CCC(C)O1	cyclohexane	-5.16	-7.96	-9.09
15-crown-5	C1OCCOCCOCCOCCO1	cyclohexane	-10.01	-15.01	-18.28
methanol	CO	cyclohexane	-1.64	-4.04	-3.65
ethanol	CCO	cyclohexane	-2.43	-4.18	-4.97
isopropanol	CC(C)O	cyclohexane	-2.99	-4.97	-5.90
1-hexanol	CCCCCCO	cyclohexane	-5.32	-8.70	-9.57
1-octanol	CCCCCCCCO	cyclohexane	-6.71	-11.09	-11.79
1-nonanol	CCCCCCCCCO	cyclohexane	-7.50	-12.88	-13.06
1-decanol	CCCCCCCCCO	cyclohexane	-8.09	-13.45	-14.12
2-methoxyethanol	COCCO	cyclohexane	-4.07	-7.78	-8.11
2-ethoxyethanol	CCOCCO	cyclohexane	-4.95	-8.58	-9.42
methyl acetate	COC(C)=O	cyclohexane	-3.51	-5.72	-6.61
ethyl acetate	CCOC(C)=O	cyclohexane	-4.05	-6.66	-7.43
propyl acetate	CCCOC(C)=O	cyclohexane	-4.71	-7.70	-8.46
methyl propanoate	CCC(=O)OC	cyclohexane	-4.11	-6.60	-7.52
propyl propionate	CCCOC(=O)CC	cyclohexane	-5.29	-9.13	-9.38
methyl benzoate	COC(=O)c1ccccc1	cyclohexane	-6.99	-11.19	-11.94
propyl benzoate	CCCOC(=O)c1ccccc1	cyclohexane	-8.21	-13.70	-13.89
butyl benzoate	CCCCOC(=O)c1ccccc1	cyclohexane	-8.90	-14.67	-14.96
acetonitrile	CC#N	cyclohexane	-2.99	-4.29	-5.04
propionitrile	CCC#N	cyclohexane	-3.64	-5.62	-6.01
benzene	c1ccccc1	cyclohexane	-4.24	-7.33	-7.64
ethylbenzene	CCc1ccccc1	cyclohexane	-5.58	-9.42	-9.66
sec-butylbenzene	CCC(C)c1ccccc1	cyclohexane	-6.86	-11.27	-11.62
1,2-dimethylbenzene	Cc1ccccc1C	cyclohexane	-5.54	-9.61	-9.63
1,3-dimethylbenzene	Cc1cccc(C)c1	cyclohexane	-5.53	-9.44	-9.61
1,4-dimethylbenzene	Cc1ccc(C)cc1	cyclohexane	-5.54	-9.27	-9.61
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	cyclohexane	-6.16	-10.36	-10.57
1,2,4,5-tetramethylbenzene	Cc1cc(C)c(C)cc1C	cyclohexane	-6.79	-11.76	-11.56
hexamethylbenzene	Cc1c(C)c(C)c(C)c(C)c1C	cyclohexane	-7.92	-14.36	-13.33
cyclohexylbenzene	C1CCC(CC1)c2ccccc2	cyclohexane	-8.50	-13.76	-13.94
naphthalene	c1ccc2ccccc2c1	cyclohexane	-7.33	-11.92	-12.55
biphenyl	c1ccc(cc1)c2ccccc2	cyclohexane	-8.71	-13.81	-14.59
anthracene	c1ccc2cc3ccccc3cc2c1	cyclohexane	-10.33	-17.21	-17.23
fluorene	C1c2ccccc2c3ccccc13	cyclohexane	-9.61	-14.60	-15.97
acenaphthene	C1Cc2ccccc2c1c23	cyclohexane	-8.86	-13.71	-14.76
1-methylnaphthalene	Cc1cccc2ccccc12	cyclohexane	-7.99	-13.15	-13.56
4-methylbiphenyl	Cc1ccc(cc1)c2ccccc2	cyclohexane	-9.33	-14.03	-15.51
1,2-diphenylethane	C(Cc1ccccc1)c2ccccc2	cyclohexane	-10.14	-15.37	-16.72
anisole	COc1ccccc1	cyclohexane	-5.61	-9.47	-9.66
benzaldehyde	O=Cc1ccccc1	cyclohexane	-5.83	-9.54	-9.95
benzonitrile	N#Cc1ccccc1	cyclohexane	-6.36	-9.74	-10.23
1,2-dichlorobenzene	Clc1ccccc1Cl	cyclohexane	-6.30	-10.15	-10.70
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	cyclohexane	-6.45	-10.21	-10.90
hexachlorobenzene	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	cyclohexane	-9.70	-15.49	-16.09
fluorobenzene	Fc1ccccc1	cyclohexane	-4.18	-7.39	-7.56
1,4-difluorobenzene	Fc1ccc(F)cc1	cyclohexane	-4.43	-7.39	-8.05
hexafluorobenzene	Fc1c(F)c(F)c(F)c(F)c1F	cyclohexane	-3.03	-6.49	-6.94
iodobenzene	Ic1ccccc1	cyclohexane	-6.50	-10.54	-10.51
nitrobenzene	[O-][N+](=O)c1ccccc1	cyclohexane	-6.17	-10.30	-10.86
trifluoromethylbenzene	FC(F)(F)c1ccccc1	cyclohexane	-4.56	-7.32	-7.92
<i>N</i> -methylpyrrole	Cn1ccccc1	cyclohexane	-4.84	-7.81	-8.69
aniline	Nc1ccccc1	cyclohexane	-5.89	-9.11	-10.03
<i>N</i> -ethylaniline	CCNc1ccccc1	cyclohexane	-6.92	-11.58	-12.04
<i>N,N</i> -dimethylaniline	CN(C)c1ccccc1	cyclohexane	-6.76	-11.09	-11.76
methyl methacrylate	COC(=O)C(C)=C	cyclohexane	-4.65	-7.30	-8.33
nitromethane	C[N+](=[O-])=O	cyclohexane	-3.06	-6.12	-6.13
nitroethane	CC[N+](=[O-])=O	cyclohexane	-3.77	-6.79	-7.28
1-nitropropane	CCC[N+](=[O-])=O	cyclohexane	-4.44	-7.89	-8.30
2-nitropropane	CC(C)[N+](=[O-])=O	cyclohexane	-4.42	-7.23	-8.30
helium	[He]	cyclohexane	1.95	2.42	1.91
neon	[Ne]	cyclohexane	1.80	1.46	1.57
krypton	[Kr]	cyclohexane	-0.10	-0.85	-0.99
xenon	[Xe]	cyclohexane	-1.05	-2.39	-2.49
hydrogen	[H][H]	cyclohexane	1.45	1.24	1.08
carbon monoxide	C=O	cyclohexane	0.65	0.20	0.02
carbon dioxide	O=C=O	cyclohexane	-0.10	-1.59	-1.17
oxygen	O=O	cyclohexane	0.80	0.06	0.23
carbon tetrafluoride	FC(F)(F)F	cyclohexane	0.79	0.12	-0.10
sulfur hexafluoride	F[S](F)(F)(F)(F)F	cyclohexane	-0.02	-1.38	-1.35
sulfur dioxide	O=[S]=O	cyclohexane	-2.26	-3.50	-4.66
pyridine	c1ccncc1	cyclohexane	-4.75	-7.65	-8.03
4-methylpyridine	Cc1ccncc1	cyclohexane	-5.49	-8.87	-9.21
2,6-dimethylpyridine	Cc1cccc(C)n1	cyclohexane	-6.19	-9.53	-10.45



2-chloropyridine	<chem>Clc1cccn1</chem>	cyclohexane	-6.09	-9.49	-10.27
3-cyanopyridine	<chem>N#Cc1cccn1</chem>	cyclohexane	-7.10	-9.68	-11.33
4-cyanopyridine	<chem>N#Cc1cncn1</chem>	cyclohexane	-7.01	-9.27	-11.11
1-butanethiol	<chem>CCCCS</chem>	cyclohexane	-4.96	-7.96	-8.20
dimethylformamide	<chem>CN(C)C=O</chem>	cyclohexane	-4.90	-8.15	-9.31
n-butylamine	<chem>CCCCN</chem>	cyclohexane	-3.73	-7.05	-7.04
sec-butylamine	<chem>CCC(C)N</chem>	cyclohexane	-3.33	-6.38	-6.59
tert-butylamine	<chem>CC(C)(C)N</chem>	cyclohexane	-3.21	-6.07	-6.60
heptylamine	<chem>CCCCCCCN</chem>	cyclohexane	-5.91	-10.49	-10.71
octylamine	<chem>CCCCCCCCN</chem>	cyclohexane	-6.57	-11.77	-11.76
nonylamine	<chem>CCCCCCCCCN</chem>	cyclohexane	-7.56	-12.76	-13.32
cyclohexylamine	<chem>NC1CCCCC1</chem>	cyclohexane	-5.37	-9.03	-9.47
diethylamine	<chem>CCNCC</chem>	cyclohexane	-3.85	-6.98	-7.57
dipropylamine	<chem>CCCNCCC</chem>	cyclohexane	-5.09	-9.13	-9.66
dibutylamine	<chem>CCCCNCCCC</chem>	cyclohexane	-6.28	-11.11	-11.68
triethylamine	<chem>CCN(CC)CC</chem>	cyclohexane	-4.72	-8.08	-8.77
tripropylamine	<chem>CCCN(CCC)CCC</chem>	cyclohexane	-6.60	-10.64	-11.91
tri-n-butylamine	<chem>CCCCN(CCCC)CCCC</chem>	cyclohexane	-8.37	-16.14	-14.90
carbon disulfide	<chem>S=C=S</chem>	cyclohexane	-4.07	-6.24	-5.64
2-bromo-2-methylpropane	<chem>CC(C)(C)Br</chem>	cyclohexane	-4.18	-7.04	-7.53
1-adamantanol	<chem>OC12CC3CC(CC(C3)C1)C2</chem>	cyclohexane	-8.69	-13.77	-14.30
1-chloroadamantane	<chem>ClC12CC3CC(CC(C3)C1)C2</chem>	cyclohexane	-8.75	-13.00	-14.04
2-chloroadamantane	<chem>ClC1C2CC3CC(C2)CC1C3</chem>	cyclohexane	-8.83	-13.67	-14.00
2-bromoadamantane	<chem>BrC1C2CC3CC(C2)CC1C3</chem>	cyclohexane	-8.92	-14.53	-14.21
1-chloro-2-nitrobenzene	<chem>[O-][N+](=O)c1ccccc1Cl</chem>	cyclohexane	-6.82	-11.90	-11.85
salicylaldehyde	<chem>Oc1ccccc1C=O</chem>	cyclohexane	-6.76	-9.92	-11.63
tetramethylstannane	<chem>C[Sn](C)(C)C</chem>	cyclohexane	-4.15	-7.36	-7.01
N-methylimidazole	<chem>Cn1ccn1</chem>	cyclohexane	-5.83	-9.07	-10.02
methane	<chem>C</chem>	benzene	-0.19	-0.30	-1.00
ethane	<chem>CC</chem>	benzene	-1.00	-2.00	-2.21
propane	<chem>CCC</chem>	benzene	-1.71	-3.20	-3.32
isobutane	<chem>CC(C)C</chem>	benzene	-2.33	-3.70	-4.28
butane	<chem>CCCC</chem>	benzene	-2.37	-4.16	-4.34
pentane	<chem>CCCCC</chem>	benzene	-3.12	-5.29	-5.51
heptane	<chem>CCCCCCC</chem>	benzene	-4.54	-7.41	-7.74
octane	<chem>CCCCCCCC</chem>	benzene	-5.30	-8.48	-9.00
decane	<chem>CCCCCCCCC</chem>	benzene	-6.69	-10.48	-11.12
undecane	<chem>CCCCCCCCCCC</chem>	benzene	-7.35	-11.95	-12.21
dodecane	<chem>CCCCCCCCCCCC</chem>	benzene	-8.08	-12.50	-13.38
tetradecane	<chem>CCCCCCCCCCCCC</chem>	benzene	-9.46	-14.73	-15.56
hexadecane	<chem>CCCCCCCCCCCCCCC</chem>	benzene	-10.88	-16.75	-17.80
2-methylbutane	<chem>CCC(C)C</chem>	benzene	-3.02	-4.90	-5.34
3-ethylpentane	<chem>CCC(CC)CC</chem>	benzene	-4.37	-7.17	-7.45
2,2-dimethylbutane	<chem>CCC(C)(C)C</chem>	benzene	-3.75	-5.47	-6.81
2,2-dimethylpentane	<chem>CCCC(C)(C)C</chem>	benzene	-4.44	-6.44	-7.87
3,3-diethylpentane	<chem>CCC(CC)(CC)CC</chem>	benzene	-5.76	-8.81	-9.97
2-methyloctane	<chem>CCCCCCC(C)C</chem>	benzene	-5.83	-9.09	-9.81
2,2,4-trimethylpentane	<chem>CC(C)CC(C)(C)C</chem>	benzene	-5.03	-6.97	-8.79
2,2,4,4-tetramethylpentane	<chem>CC(C)(C)CC(C)(C)C</chem>	benzene	-5.30	-7.65	-9.23
cyclohexane	<chem>C1CCCCC1</chem>	benzene	-4.20	-7.03	-7.03
cycloheptane	<chem>C1CCCCC1</chem>	benzene	-4.91	-8.45	-8.14
cyclooctane	<chem>C1CCCCC1</chem>	benzene	-5.59	-9.48	-9.20
methylcyclohexane	<chem>CC1CCCCC1</chem>	benzene	-4.83	-7.48	-8.02
cis-1,2-dimethylcyclohexane	<chem>C[C@H]1CCCC[C@H]1C</chem>	benzene	-5.44	-8.43	-8.98
ethene	<chem>C=C</chem>	benzene	-1.04	-2.15	-2.25
1-butene	<chem>CCC=C</chem>	benzene	-2.50	-4.43	-4.54
cis-2-butene	<chem>C/C=C/C</chem>	benzene	-2.63	-5.01	-4.83
trans-2-butene	<chem>C/C=C/C</chem>	benzene	-2.59	-4.60	-4.72
isobutene	<chem>CC(C)=C</chem>	benzene	-2.54	-4.57	-4.67
1-pentene	<chem>CCCC=C</chem>	benzene	-3.14	-5.48	-5.50
1-hexene	<chem>CCCCC=C</chem>	benzene	-3.89	-6.67	-6.69
1-heptene	<chem>CCCCC=C</chem>	benzene	-4.57	-7.76	-7.76
1-octene	<chem>CCCCC=C</chem>	benzene	-5.31	-8.77	-8.92
1-nonene	<chem>CCCCC=C</chem>	benzene	-6.00	-9.85	-10.02
1-dodecene	<chem>CCCCCCCCC=C</chem>	benzene	-8.11	-13.03	-13.46
1-tetradecene	<chem>CCCCCCCCCCCCC=C</chem>	benzene	-9.51	-15.16	-15.61
1-pentadecene	<chem>CCCCCCCCCCCCC=C</chem>	benzene	-10.21	-16.21	-16.79
cis-2-octene	<chem>CCCCC=C/C</chem>	benzene	-5.39	-8.60	-9.10
trans-2-octene	<chem>CCCCC/C=C/C</chem>	benzene	-5.34	-8.56	-9.01
cis-4-octene	<chem>CCC/C=C/CCC</chem>	benzene	-5.34	-8.47	-9.01
1,5-hexadiene	<chem>C=CCCC=C</chem>	benzene	-3.97	-6.98	-6.83
cyclopentene	<chem>C1CC=CC1</chem>	benzene	-3.78	-6.28	-6.62
cyclohexene	<chem>C1CCC=CC1</chem>	benzene	-4.38	-7.53	-7.43
norbornadiene	<chem>C1CC2=CC=C1C2</chem>	benzene	-5.39	-8.04	-8.98
acetone	<chem>CC(C)=O</chem>	benzene	-3.71	-7.19	-6.89
2-pentanone	<chem>CCCC(C)=O</chem>	benzene	-5.08	-8.99	-8.99
3-pentanone	<chem>CCC(=O)CC</chem>	benzene	-5.10	-9.22	-9.02
2-hexanone	<chem>CCCCC(C)=O</chem>	benzene	-5.76	-10.08	-10.04
2-heptanone	<chem>CCCCC(C)=O</chem>	benzene	-6.41	-11.10	-11.03
4-heptanone	<chem>CCCC(=O)CCC</chem>	benzene	-6.32	-10.95	-10.87
2-octanone	<chem>CCCCCCC(C)=O</chem>	benzene	-7.08	-12.15	-12.06
2-nonanone	<chem>CCCCCCC(C)=O</chem>	benzene	-7.64	-13.14	-12.86
5-nonanone	<chem>CCCCC(=O)CCCC</chem>	benzene	-7.58	-12.75	-12.76

6-undecanone	CCCCC(=O)CCCC	benzene	-8.67	-14.67	-14.44
tert-butyl methyl ketone	CC(=O)C(C)C	benzene	-5.27	-9.00	-9.33
di-tert-butyl ketone	CC(C)(C)C(=O)C(C)C	benzene	-6.42	-10.28	-11.00
cyclopentanone	O=C1CCCC1	benzene	-5.58	-10.45	-9.79
cycloheptanone	O=C1CCCCC1	benzene	-6.84	-11.86	-11.65
methyl butyl ether	CCCCOC	benzene	-4.49	-7.50	-7.90
methyl heptyl ether	CCCCCCCOC	benzene	-6.39	-10.71	-10.74
methyl tert-butyl ether	COC(C)(C)C	benzene	-4.24	-6.70	-7.64
methyl tert-amyl ether	CCC(C)(C)OC	benzene	-4.71	-8.27	-8.30
tetrahydrofuran	C1CCOC1	benzene	-4.49	-7.60	-8.02
1,4-dioxane	C1COCCO1	benzene	-5.25	-9.33	-9.35
dimethoxymethane	COCOC	benzene	-4.10	-6.72	-7.45
1,2-dimethoxyethane	COCOC	benzene	-4.85	-8.89	-8.52
diglyme	COCCOCCOC	benzene	-6.85	-11.71	-11.67
12-crown-4	C1COCCOCCOCCO1	benzene	-8.87	-15.77	-15.99
15-crown-5	C1COCCOCCOCCOCCO1	benzene	-10.70	-19.47	-19.46
18-crown-6	C1COCCOCCOCCOCCOCCO1	benzene	-13.00	-24.09	-23.78
1-butanol	CCCCO	benzene	-4.31	-8.40	-7.95
1-pentanol	CCCCCO	benzene	-4.93	-9.40	-8.88
1-hexanol	CCCCCCO	benzene	-5.74	-11.87	-10.16
1-octanol	CCCCCCCCO	benzene	-7.06	-12.61	-12.24
1-decanol	CCCCCCCCCO	benzene	-8.33	-15.54	-14.34
tert-butanol	CC(C)(C)O	benzene	-4.12	-8.13	-7.94
2-methyl-2-butanol	CCC(C)(C)O	benzene	-4.69	-8.00	-8.82
2-ethoxyethanol	COCCO	benzene	-5.61	-9.42	-10.50
1,1-difluoroethane	CC(F)F	benzene	-2.13	-4.33	-4.27
1-fluorooctane	CCCCCCCCF	benzene	-6.51	-11.38	-11.23
1-chlorohexane	CCCCCCCl	benzene	-5.71	-10.03	-9.77
1-chlorooctane	CCCCCCCCCl	benzene	-7.02	-12.04	-11.76
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	benzene	-6.51	-11.41	-10.77
tetrachloromethane	ClC(Cl)(Cl)Cl	benzene	-4.73	-7.62	-8.09
chloroform	ClC(Cl)Cl	benzene	-4.27	-7.71	-7.34
phenol	Oc1ccccc1	benzene	-6.09	-11.94	-10.72
2,6-dimethylphenol	Cc1ccc(C)c1O	benzene	-7.38	-12.57	-12.82
1-naphthol	Oc1cccc2ccccc12	benzene	-9.37	-16.54	-16.08
dimethyl sulfoxide	C[S](C)=O	benzene	-6.65	-11.49	-11.85
pyridine	c1ccncc1	benzene	-5.34	-9.61	-8.95
2-methylpyridine	Cc1cccn1	benzene	-6.12	-10.14	-10.25
3-methylpyridine	Cc1cccn1	benzene	-6.10	-10.54	-10.17
2,4-dimethylpyridine	Cc1cnc(C)c1	benzene	-6.88	-11.24	-11.52
2,6-dimethylpyridine	Cc1ccc(C)n1	benzene	-6.84	-10.76	-11.49
2-fluoropyridine	Fc1cccn1	benzene	-5.42	-9.82	-9.53
2-iodopyridine	Ic1cccn1	benzene	-8.22	-13.18	-13.18
2-chloropyridine	Clc1cccn1	benzene	-6.77	-11.45	-11.42
3-chloropyridine	Clc1cccn1	benzene	-6.85	-11.59	-11.50
3-cyanopyridine	N#Cc1cccn1	benzene	-8.10	-12.93	-12.91
4-cyanopyridine	N#Cc1cccn1	benzene	-8.00	-13.15	-12.68
butylamine	CCCCN	benzene	-4.12	-7.82	-7.48
sec-butylamine	CCC(C)N	benzene	-3.57	-7.43	-6.85
hexylamine	CCCCCN	benzene	-5.39	-10.21	-9.70
cyclohexylamine	NC1CCCCC1	benzene	-5.51	-9.75	-9.46
diethylamine	CCNCC	benzene	-4.01	-7.60	-7.60
dipropylamine	CCCNCCC	benzene	-5.24	-9.51	-9.72
dibutylamine	CCCCNCCCC	benzene	-6.36	-11.23	-11.67
triethylamine	CCN(CC)CC	benzene	-4.83	-8.86	-8.74
nitric oxide	[N]=O	benzene	0.19	0.59	-0.38
helium	[He]	benzene	1.88	2.46	1.93
neon	[Ne]	benzene	1.84	2.50	1.69
argon	[Ar]	benzene	0.48	0.30	-0.13
krypton	[Kr]	benzene	-0.11	-0.46	-0.80
xenon	[Xe]	benzene	-1.10	-1.70	-2.35
radon	[Rn]	benzene	-1.26	-3.18	-2.54
hydrogen	[H][H]	benzene	1.38	1.52	1.13
carbon monoxide	C=O	benzene	0.41	0.64	-0.19
carbon dioxide	O=C=O	benzene	-0.62	-2.20	-1.94
oxygen	O=O	benzene	0.58	0.41	0.07
tetrafluoromethane	FC(F)(F)F	benzene	1.01	0.54	0.45
sulfur hexafluoride	F[S](F)(F)(F)F	benzene	0.23	-0.78	-0.82
benzene	c1ccccc1	benzene	-4.61	-8.09	-8.08
toluene	Cc1ccccc1	benzene	-5.32	-9.00	-9.18
1,4-dimethylbenzene	Cc1ccc(C)cc1	benzene	-5.97	-10.07	-10.20
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	benzene	-6.60	-10.70	-11.18
naphthalene	c1ccc2ccccc2c1	benzene	-7.82	-13.21	-13.19
phenanthrene	c1ccc2c(c1)ccc3ccccc23	benzene	-10.89	-17.70	-18.03
biphenyl	c1ccc(cc1)c2ccccc2	benzene	-9.21	-15.15	-15.24
anthracene	c1ccc2cc3ccccc3cc2c1	benzene	-10.91	-18.69	-18.09
anisole	COc1ccccc1	benzene	-6.25	-11.13	-10.72
γ-butyrolactone	O=C1CCCOC1	benzene	-6.12	-12.89	-11.11
ethyl formate	CCOC=O	benzene	-4.13	-7.26	-7.62
methyl acetate	COC(C)=O	benzene	-4.34	-7.55	-8.02
ethyl acetate	CCOC(C)=O	benzene	-4.77	-8.30	-8.66
propyl acetate	CCCOC(C)=O	benzene	-5.40	-9.31	-9.62
butyl acetate	CCCCOC(C)=O	benzene	-5.96	-10.30	-10.42

ethyl benzoate	CCOC(=O)c1ccccc1	benzene	-8.33	-14.05	-14.12
propyl benzoate	CCCOC(=O)c1ccccc1	benzene	-8.89	-15.37	-14.93
difluorodichloromethane	FC(F)(Cl)Cl	benzene	-1.87	-4.44	-3.98
1-butanethiol	CCCCS	benzene	-5.42	-8.55	-8.93
methyl methacrylate	COC(=O)C(C)=C	benzene	-5.34	-9.19	-9.46
benzonitrile	N#Cc1ccccc1	benzene	-7.25	-12.44	-11.75
chlorotrifluoromethane	FC(F)(F)Cl	benzene	-0.34	-1.20	-1.65
diiodomethane	ICI	benzene	-6.72	-10.76	-10.49
nitrobenzene	[O-][N+](=O)c1ccccc1	benzene	-7.03	-12.60	-12.38
trifluoromethylbenzene	FC(F)(F)c1ccccc1	benzene	-4.80	-8.40	-8.06
3-methylphenol	Cc1ccc(O)c1	benzene	-6.82	-12.20	-11.92
acetonitrile	CC#N	benzene	-3.94	-7.46	-6.67
propionitrile	CCC#N	benzene	-4.54	-8.70	-7.52
butanenitrile	CCCC#N	benzene	-5.11	-9.32	-8.38
1-nitropropane	CCC[N+](=[O-])=O	benzene	-5.47	-10.37	-10.11
2-nitropropane	CC(C)[N+](=[O-])=O	benzene	-5.44	-9.63	-10.12
nitromethane	C[N+](=[O-])=O	benzene	-4.08	-8.37	-7.95
nitroethane	CC[N+](=[O-])=O	benzene	-4.80	-9.15	-9.10
fluorobenzene	Fc1ccccc1	benzene	-4.66	-8.47	-8.20
chlorobenzene	Clc1ccccc1	benzene	-5.76	-9.76	-9.79
1,3-dichlorobenzene	Clc1cccc(Cl)c1	benzene	-6.97	-10.98	-11.68
bromobenzene	Brc1ccccc1	benzene	-6.03	-10.42	-10.21
1,2-dibromobenzene	Brc1ccccc1Br	benzene	-7.54	-12.70	-12.58
1,3-dibromobenzene	Brc1cccc(Br)c1	benzene	-7.66	-12.64	-12.80
iodobenzene	Ic1ccccc1	benzene	-7.09	-11.65	-11.44
1,2-diiodobenzene	Ic1cccc(I)c1	benzene	-9.56	-15.16	-14.77
1,3-diiodobenzene	Ic1cccc(I)c1	benzene	-9.72	-15.08	-15.07
1,4-diiodobenzene	Ic1ccc(I)cc1	benzene	-9.72	-15.20	-15.07
2-bromotoluene	Cc1cccc1Br	benzene	-6.65	-11.16	-11.11
3-bromotoluene	Cc1ccc(Br)c1	benzene	-6.72	-11.28	-11.29
4-bromotoluene	Cc1ccc(Br)cc1	benzene	-6.73	-11.64	-11.30
2-iodotoluene	Cc1cccc1I	benzene	-7.85	-12.14	-12.65
3-iodotoluene	Cc1cccc(I)c1	benzene	-7.83	-12.25	-12.64
aniline	Nc1ccccc1	benzene	-6.67	-12.08	-11.42
benzaldehyde	O=Cc1ccccc1	benzene	-6.62	-11.70	-11.28
1-bromonaphthalene	Brc1cccc2ccccc12	benzene	-9.09	-14.98	-15.01
1-iodonaphthalene	Ic1cccc2ccccc12	benzene	-10.19	-16.30	-16.34
4-bromobiphenyl	Brc1ccc(cc1)c2ccccc2	benzene	-10.45	-16.95	-16.98
4,4'-dibromobiphenyl	Brc1ccc(cc1)c2ccc(Br)cc2	benzene	-11.94	-19.69	-19.27
1,2-dicyanobenzene	N#Cc1ccccc1C#N	benzene	-9.44	-16.06	-14.97
4-nitrotoluene	Cc1ccc(cc1)[N+](=[O-])=O	benzene	-7.80	-14.66	-13.60
2,4-dinitrotoluene	Cc1ccc(cc1[N+](=[O-])=O)[N+](=[O-])=O	benzene	-9.78	-17.83	-17.21
pyrrole	[nH]1ccccc1	benzene	-5.10	-10.06	-8.88
N-methylpyrrole	Cn1ccccc1	benzene	-5.24	-9.57	-9.14
1-bromo-4-chlorobenzene	Clc1ccc(Br)cc1	benzene	-7.33	-12.03	-12.30
2-chloroaniline	Nc1ccccc1Cl	benzene	-8.06	-13.17	-13.62
1-chloro-2-nitrobenzene	[O-][N+](=O)c1ccccc1Cl	benzene	-7.61	-14.44	-13.21
1-chloro-4-nitrobenzene	[O-][N+](=O)c1ccc(Cl)cc1	benzene	-8.02	-14.24	-13.85
1-aminonaphthalene	Nc1cccc2ccccc12	benzene	-9.75	-16.49	-16.38
2-nitroaniline	Nc1ccccc1[N+](=[O-])=O	benzene	-9.05	-15.99	-15.97
o-phenylenediamine	Nc1ccccc1N	benzene	-8.08	-15.11	-14.66
p-phenylenediamine	Nc1ccc(N)cc1	benzene	-9.05	-16.32	-15.94
1-nitropyrene	[O-][N+](=O)c1ccc2ccc3ccccc3cc1c2c34	benzene	-14.82	-24.76	-24.70
dimethyl terephthalate	COC(=O)c1ccc(cc1)C(=O)OC	benzene	-10.53	-17.97	-17.83
water	O	benzene	-1.94	-4.68	-4.56
2-chlorophenol	Oc1ccccc1Cl	benzene	-6.81	-11.35	-11.59
2-nitrophenol	Oc1ccccc1[N+](=[O-])=O	benzene	-7.29	-12.26	-12.91
2'-hydroxyacetophenone	CC(=O)c1ccccc1O	benzene	-8.72	-13.48	-15.29
2-hydroxybenzaldehyde	Oc1ccccc1C=O	benzene	-6.76	-12.33	-11.51
2,3-dimethoxyphenol	COc1ccc(O)c1OC	benzene	-8.63	-16.56	-15.37
4-nitro-2-methoxyphenol	COc1cc(ccc1O)[N+](=[O-])=O	benzene	-9.90	-18.09	-17.94
2,6-dichlorophenol	Oc1c(Cl)cccc1Cl	benzene	-7.92	-12.55	-13.22
2,4,6-trichlorophenol	Oc1c(Cl)cc(Cl)cc1Cl	benzene	-8.91	-14.15	-14.66
4-methoxy-2-nitrophenol	COc1ccc(O)c(c1)[N+](=[O-])=O	benzene	-9.41	-16.09	-16.84
methyl isonicotinate	COC(=O)c1ccncc1	benzene	-9.23	-14.24	-15.89
salicylaldehyde	Oc1ccccc1C=O	benzene	-7.88	-11.99	-13.74
tetramethylstannane	C[Sn](C)(C)C	benzene	-3.93	-6.70	-6.21
5-chloro-1,10-phenanthroline	Clc1cc2ccccc2c3ncccc13	benzene	-13.77	-22.37	-22.35
butane	CCCC	dimethyl sulfoxide	-0.61	-2.89	-3.20
pentane	CCCCC	dimethyl sulfoxide	-1.24	-3.64	-4.20
hexane	CCCCCC	dimethyl sulfoxide	-1.85	-4.21	-5.18
octane	CCCCCCCC	dimethyl sulfoxide	-2.89	-5.76	-6.92
nonane	CCCCCCCCC	dimethyl sulfoxide	-3.47	-6.61	-7.78
decane	CCCCCCCCC	dimethyl sulfoxide	-4.24	-7.36	-9.03
cyclohexane	C1CCCCC1	dimethyl sulfoxide	-2.51	-5.16	-6.08
1-butene	CCC=C	dimethyl sulfoxide	-1.21	-3.70	-4.27
1-pentene	CCCC=C	dimethyl sulfoxide	-1.79	-4.85	-5.11
1-hexene	CCCCC=C	dimethyl sulfoxide	-2.35	-5.14	-5.95
1-octene	CCCCCCC=C	dimethyl sulfoxide	-3.43	-7.60	-7.61
1-octyne	CCCCCCCC#C	dimethyl sulfoxide	-4.00	-8.88	-8.61
2-octyne	CCCCC#CC	dimethyl sulfoxide	-4.20	-8.93	-8.98
benzene	c1ccccc1	dimethyl sulfoxide	-3.24	-7.34	-7.18

1,3-dimethylbenzene	Cc1cccc(C)c1	dimethyl sulfoxide	-4.48	-9.98	-9.21
1,4-dimethylbenzene	Cc1ccc(C)cc1	dimethyl sulfoxide	-4.49	-9.00	-9.22
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	dimethyl sulfoxide	-5.04	-9.41	-10.13
butylbenzene	CCCCc1ccccc1	dimethyl sulfoxide	-5.65	-10.20	-10.98
pentylbenzene	CCCCC1CCCCC1	dimethyl sulfoxide	-6.22	-10.86	-11.90
hexylbenzene	CCCCCc1ccccc1	dimethyl sulfoxide	-6.86	-11.64	-12.97
octylbenzene	CCCCCCCCc1ccccc1	dimethyl sulfoxide	-8.21	-12.70	-15.19
naphthalene	c1ccc2ccccc2c1	dimethyl sulfoxide	-6.29	-12.71	-11.92
biphenyl	c1ccc(cc1)c2ccccc2	dimethyl sulfoxide	-7.99	-14.57	-14.42
anthracene	c1ccc2cc3ccccc3cc2c1	dimethyl sulfoxide	-9.88	-18.31	-17.60
methylamine	CN	dimethyl sulfoxide	-1.95	-6.41	-6.12
n-propylamine	CCCN	dimethyl sulfoxide	-2.71	-7.23	-8.12
n-butylamine	CCCCN	dimethyl sulfoxide	-3.50	-8.03	-9.37
n-pentylamine	CCCCCN	dimethyl sulfoxide	-4.36	-8.72	-11.05
n-hexylamine	CCCCCCN	dimethyl sulfoxide	-4.49	-9.66	-11.41
ethylenediamine	NCCN	dimethyl sulfoxide	-7.01	-9.97	-16.23
triethylamine	CCN(CC)CC	dimethyl sulfoxide	-3.02	-6.29	-8.24
methyl ethyl ketone	CCC(C)=O	dimethyl sulfoxide	-3.48	-7.76	-7.57
2-hexanone	CCCCC(C)=O	dimethyl sulfoxide	-4.49	-9.51	-9.15
4-heptanone	CCCC(=O)CCC	dimethyl sulfoxide	-5.13	-9.52	-10.26
2-nonanone	CCCCCCCC(C)=O	dimethyl sulfoxide	-6.11	-11.28	-11.76
5-nonanone	CCCCC(=O)CCCC	dimethyl sulfoxide	-5.98	-10.71	-11.56
di-tert-butylketone	CC(C)(C)C(=O)C(C)(C)C	dimethyl sulfoxide	-4.41	-8.40	-9.36
cyclohexanone	O=C1CCCCC1	dimethyl sulfoxide	-5.14	-10.00	-10.16
diethyl ether	CCOCC	dimethyl sulfoxide	-2.36	-5.16	-5.78
dipropyl ether	CCCOCCC	dimethyl sulfoxide	-3.52	-7.07	-7.64
dibutyl ether	CCCCOCCCC	dimethyl sulfoxide	-4.56	-7.65	-9.41
ethyl propyl ether	CCCOCC	dimethyl sulfoxide	-2.94	-6.03	-6.65
n-butyl methyl ether	CCCCOC	dimethyl sulfoxide	-2.97	-6.06	-6.78
methyl heptyl ether	CCCCCCCOC	dimethyl sulfoxide	-4.69	-8.70	-9.57
methyl tert-amyl ether	CCC(C)(C)OC	dimethyl sulfoxide	-3.03	-6.95	-7.14
tetrahydrofuran	C1CCOC1	dimethyl sulfoxide	-3.18	-6.53	-7.16
tetrahydropyran	C1CCOCC1	dimethyl sulfoxide	-3.65	-7.21	-7.84
1,4-dioxane	C1COCCO1	dimethyl sulfoxide	-4.25	-8.75	-8.95
1,2-dimethoxyethane	COCCOC	dimethyl sulfoxide	-4.17	-8.30	-8.83
12-crown-4	C1COCCOCCOCCO1	dimethyl sulfoxide	-8.55	-15.77	-17.93
18-crown-6	C1COCCOCCOCCOCCOCCO1	dimethyl sulfoxide	-12.26	-24.82	-25.53
1-fluorooctane	CCCCCCCCF	dimethyl sulfoxide	-4.95	-8.96	-9.82
dichloromethane	CICCl	dimethyl sulfoxide	-2.58	-8.19	-6.49
chloroform	ClC(Cl)Cl	dimethyl sulfoxide	-3.39	-8.79	-7.88
tetrachloromethane	ClC(Cl)(Cl)Cl	dimethyl sulfoxide	-3.39	-7.74	-7.95
1-chlorobutane	CCCCCl	dimethyl sulfoxide	-3.32	-6.62	-7.58
2-chloro-2-methylpropane	CC(C)(C)Cl	dimethyl sulfoxide	-2.65	-5.43	-6.33
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	dimethyl sulfoxide	-4.83	-7.18	-10.05
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	dimethyl sulfoxide	-6.35	-13.58	-12.55
methyl iodide	CI	dimethyl sulfoxide	-2.67	-6.31	-6.37
1-iodobutane	CCCCI	dimethyl sulfoxide	-4.35	-8.00	-8.81
fluorobenzene	Fc1ccccc1	dimethyl sulfoxide	-3.77	-8.23	-8.03
1,2-difluorobenzene	Fc1ccccc1F	dimethyl sulfoxide	-3.67	-8.35	-8.05
1,3-difluorobenzene	Fc1cccc(F)c1	dimethyl sulfoxide	-4.67	-8.22	-9.55
4-fluorotoluene	Cc1ccc(F)cc1	dimethyl sulfoxide	-4.52	-8.84	-9.27
chlorobenzene	Clc1ccccc1	dimethyl sulfoxide	-4.61	-9.38	-9.25
1,2-dichlorobenzene	Clc1ccccc1Cl	dimethyl sulfoxide	-5.75	-11.55	-11.21
1,3-dichlorobenzene	Clc1cccc(Cl)c1	dimethyl sulfoxide	-6.10	-12.24	-11.55
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	dimethyl sulfoxide	-6.11	-10.49	-11.56
4-chlorotoluene	Cc1ccc(Cl)cc1	dimethyl sulfoxide	-5.30	-10.31	-10.39
bromobenzene	Brc1ccccc1	dimethyl sulfoxide	-4.95	-10.11	-9.73
iodobenzene	Ic1ccccc1	dimethyl sulfoxide	-5.99	-11.54	-11.06
acetonitrile	CC#N	dimethyl sulfoxide	-3.69	-7.94	-7.06
propanenitrile	CCC#N	dimethyl sulfoxide	-4.34	-8.26	-8.11
1-butanenitrile	CCCC#N	dimethyl sulfoxide	-4.95	-8.81	-9.18
1-hexanenitrile	CCCCC#N	dimethyl sulfoxide	-6.01	-10.41	-10.94
1-heptanenitrile	CCCCC#N	dimethyl sulfoxide	-6.62	-11.07	-12.05
1-nonanenitrile	CCCCCCCC#N	dimethyl sulfoxide	-7.52	-12.75	-13.35
1-decanenitrile	CCCCCCCCC#N	dimethyl sulfoxide	-8.07	-13.62	-14.31
1-dodecanenitrile	CCCCCCCCCCCC#N	dimethyl sulfoxide	-8.88	-15.13	-15.56
1-tetradecanenitrile	CCCCCCCCCCCCC#N	dimethyl sulfoxide	-9.80	-16.48	-16.98
methanol	CO	dimethyl sulfoxide	-3.10	-9.36	-8.82
isopropanol	CC(C)O	dimethyl sulfoxide	-3.84	-9.93	-10.17
1-butanol	CCCCO	dimethyl sulfoxide	-4.69	-11.51	-11.51
1-pentanol	CCCCCO	dimethyl sulfoxide	-5.03	-12.30	-11.96
1-hexanol	CCCCCCO	dimethyl sulfoxide	-5.74	-12.90	-13.02
1-octanol	CCCCCCCCO	dimethyl sulfoxide	-6.91	-14.40	-14.94
1-nonanol	CCCCCCCCCO	dimethyl sulfoxide	-7.71	-15.99	-16.24
1-decanol	CCCCCCCCCO	dimethyl sulfoxide	-7.97	-16.35	-16.82
2-methyl-isopropanol	CC(C)(C)O	dimethyl sulfoxide	-3.84	-9.64	-10.13
2-methyl-2-butanol	CCC(C)(C)O	dimethyl sulfoxide	-4.17	-10.64	-10.72
3-methyl-1-butanol	CC(C)CCO	dimethyl sulfoxide	-5.05	-12.10	-11.95
cis-1,2-cyclohexanediol	O[C@H]1CCCC[C@H]1O	dimethyl sulfoxide	-8.27	-16.66	-19.53
ethylene glycol	OCCO	dimethyl sulfoxide	-5.55	-16.65	-14.68
propylene glycol	CC(O)CO	dimethyl sulfoxide	-5.81	-15.94	-15.27
3-methylphenol	Cc1cccc(O)c1	dimethyl sulfoxide	-7.40	-17.82	-15.09
aniline	Nc1ccccc1	dimethyl sulfoxide	-6.70	-15.89	-13.15

<i>N</i> -methylaniline	CNc1ccccc1	dimethyl sulfoxide	-6.24	-13.79	-12.62
<i>N,N</i> -dimethylaniline	CN(C)c1ccccc1	dimethyl sulfoxide	-5.96	-11.78	-12.05
dimethyl carbonate	COC(=O)OC	dimethyl sulfoxide	-3.65	-8.28	-7.48
diethyl carbonate	CCOC(=O)OCC	dimethyl sulfoxide	-3.89	-9.20	-7.89
benzyl alcohol	OCc1ccccc1	dimethyl sulfoxide	-7.92	-16.80	-16.16
2-phenylethanol	OCCc1ccccc1	dimethyl sulfoxide	-8.13	-16.84	-16.34
<i>tert</i> -butyl acetate	CC(=O)OC(C)(C)C	dimethyl sulfoxide	-3.87	-8.00	-8.41
dimethylformamide	CN(C)C=O	dimethyl sulfoxide	-5.05	-10.91	-10.87
<i>N,N</i> -dimethyl acetamide	CN(C)C(C)=O	dimethyl sulfoxide	-5.48	-12.50	-11.93
acetophenone	CC(=O)c1ccccc1	dimethyl sulfoxide	-6.67	-12.27	-12.22
pyridine	c1ccncc1	dimethyl sulfoxide	-4.92	-9.32	-9.28
2,6-dimethylpyridine	Cc1ccccc1n1	dimethyl sulfoxide	-6.05	-10.18	-11.58
nitrobenzene	[O-][N+](=O)c1ccccc1	dimethyl sulfoxide	-7.33	-12.64	-13.63
(trifluoromethyl)benzene	FC(F)(F)c1ccccc1	dimethyl sulfoxide	-4.28	-7.81	-8.21
anisole	COc1ccccc1	dimethyl sulfoxide	-5.13	-10.58	-9.89
pyrrole	[nH]1ccccc1	dimethyl sulfoxide	-5.07	-13.07	-10.54
1-naphthol	Oc1ccc2ccccc12	dimethyl sulfoxide	-10.21	-21.65	-19.62
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	dimethyl sulfoxide	-7.50	-12.17	-13.79
carbon dioxide	O=C=O	dimethyl sulfoxide	-0.26	-2.97	-3.48
hexanoic acid	CCCCC(O)=O	dimethyl sulfoxide	-6.81	-17.27	-15.17
tetramethylstannane	C[Sn](C)(C)C	dimethyl sulfoxide	-2.89	-5.14	-6.54
<i>N</i> -methylimidazole	Cn1ccnc1	dimethyl sulfoxide	-6.53	-13.10	-12.57
ethane	CC	propylene carbonate	0.30	-1.37	-1.70
propane	CCC	propylene carbonate	-0.30	-1.54	-2.55
isobutane	CC(C)C	propylene carbonate	-0.77	-2.32	-3.26
butane	CCCC	propylene carbonate	-0.91	-2.59	-3.49
pentane	CCCCC	propylene carbonate	-1.50	-4.20	-4.40
hexane	CCCCCC	propylene carbonate	-2.09	-5.02	-5.32
octane	CCCCCCCC	propylene carbonate	-2.98	-7.51	-6.69
cyclohexane	C1CCCCC1	propylene carbonate	-2.40	-5.78	-5.34
methylcyclopentane	CC1CCCC1	propylene carbonate	-2.22	-5.53	-5.03
methylcyclohexane	CC1CCCCC1	propylene carbonate	-2.78	-6.27	-5.95
1-butene	CCC=C	propylene carbonate	-1.54	-4.21	-4.59
1-octene	CCCCCCC=C	propylene carbonate	-3.84	-7.30	-8.17
cyclohexene	C1CCC=CC1	propylene carbonate	-2.87	-6.46	-6.16
1,3-butadiene	C=CC=C	propylene carbonate	-2.14	-4.61	-5.68
methyl acetate	COC(C)=O	propylene carbonate	-3.98	-7.77	-8.36
ethyl acetate	CCOC(C)=O	propylene carbonate	-4.19	-8.25	-8.71
propyl acetate	CCCOC(C)=O	propylene carbonate	-4.55	-9.19	-9.36
vinyl acetate	CC(=O)OC=C	propylene carbonate	-4.21	-8.19	-8.50
butyl acetate	CCCCOC(C)=O	propylene carbonate	-4.79	-9.85	-9.76
<i>tert</i> -butyl acetate	CC(=O)OC(C)(C)C	propylene carbonate	-4.39	-8.47	-9.33
pentyl acetate	CCCCCOC(C)=O	propylene carbonate	-5.16	-10.86	-10.35
hexyl acetate	CCCCCOC(C)=O	propylene carbonate	-5.59	-11.32	-11.02
methyl propanoate	CCC(=O)OC	propylene carbonate	-4.05	-8.42	-8.41
ethyl propanoate	CCOC(=O)CC	propylene carbonate	-4.21	-9.03	-8.72
propyl propanoate	CCCOC(=O)CC	propylene carbonate	-4.66	-9.66	-9.53
methyl butanoate	CCCC(=O)OC	propylene carbonate	-4.42	-9.10	-9.08
ethyl butanoate	CCCC(=O)OCC	propylene carbonate	-4.65	-9.52	-9.49
propyl butanoate	CCCOC(=O)CCC	propylene carbonate	-5.17	-10.62	-10.40
methyl pentanoate	CCCCC(=O)OC	propylene carbonate	-4.85	-9.77	-9.78
ethyl pentanoate	CCCCC(=O)OCC	propylene carbonate	-5.17	-10.43	-10.35
ethyl hexanoate	CCCCCC(=O)OCC	propylene carbonate	-5.59	-11.54	-10.98
ethyl heptanoate	CCCCCCC(=O)OCC	propylene carbonate	-6.06	-11.38	-11.74
ethyl isobutyrate	CCOC(=O)C(C)C	propylene carbonate	-4.53	-8.99	-9.35
dimethyl carbonate	COC(=O)OC	propylene carbonate	-4.62	-8.96	-9.39
diethyl carbonate	CCOC(=O)OCC	propylene carbonate	-4.82	-10.15	-9.71
acetone	CC(C)=O	propylene carbonate	-3.04	-7.36	-6.84
methyl ethyl ketone	CCC(C)=O	propylene carbonate	-3.54	-8.19	-7.51
2-pentanone	CCCC(C)=O	propylene carbonate	-4.03	-8.99	-8.31
2-hexanone	CCCCC(C)=O	propylene carbonate	-4.52	-9.75	-9.05
2-octanone	CCCCCCC(C)=O	propylene carbonate	-5.47	-11.34	-10.52
2-undecanone	CCCCCCCCC(C)=O	propylene carbonate	-6.83	-14.13	-12.63
cyclohexanone	O=C1CCCCC1	propylene carbonate	-4.67	-10.46	-8.90
2-methylcyclohexanone	CC1CCCCC1=O	propylene carbonate	-5.16	-10.82	-9.73
anisole	COc1ccccc1	propylene carbonate	-5.74	-10.86	-10.94
phenetole	CCOc1ccccc1	propylene carbonate	-6.28	-11.38	-11.78
dimethyl sulfoxide	C[S](C)=O	propylene carbonate	-6.41	-12.29	-11.61
diethyl ether	CCOCC	propylene carbonate	-2.67	-6.09	-6.07
diisopropyl ether	CC(C)OC(C)C	propylene carbonate	-3.40	-6.92	-7.39
ethyl <i>tert</i> -butyl ether	CCOC(C)(C)C	propylene carbonate	-3.23	-7.34	-7.14
methyl <i>tert</i> -amyl ether	CCC(C)(C)OC	propylene carbonate	-3.24	-8.07	-7.17
tetrahydropyran	C1CCOCC1	propylene carbonate	-3.35	-8.21	-6.68
tetrahydrofuran	C1CCOC1	propylene carbonate	-2.79	-7.58	-5.81
1,3-dioxolane	C1COCO1	propylene carbonate	-3.38	-8.63	-6.99
12-crown-4	C1COCOCOCOCOC1	propylene carbonate	-8.05	-16.43	-16.21
15-crown-5	C1COCOCOCOCOCOC1	propylene carbonate	-9.79	-21.51	-19.76
18-crown-6	C1COCOCOCOCOCOCOC1	propylene carbonate	-12.02	-26.02	-24.14
methanol	CO	propylene carbonate	-2.67	-7.53	-7.56
propan-1-ol	CCCO	propylene carbonate	-3.65	-8.80	-9.17
butan-1-ol	CCCCO	propylene carbonate	-3.97	-9.87	-9.61
2-butanol	CCC(C)O	propylene carbonate	-3.68	-9.17	-9.09
pentan-1-ol	CCCCCO	propylene carbonate	-4.64	-10.83	-10.77

2-pentanol	CCCC(C)O	propylene carbonate	-4.10	-9.40	-9.76
3-pentanol	CCC(O)CC	propylene carbonate	-4.20	-9.48	-10.02
2-methyl-2-butanol	CCC(C)(C)O	propylene carbonate	-3.29	-9.29	-8.45
3-methyl-1-butanol	CC(C)CCO	propylene carbonate	-4.52	-9.55	-10.49
ethan-1,2-diol	OCCO	propylene carbonate	-5.80	-12.99	-14.21
2-methoxyethanol	COCCO	propylene carbonate	-4.55	-9.61	-10.84
2-ethoxyethanol	CCOCCO	propylene carbonate	-4.92	-10.14	-10.96
benzene	c1ccccc1	propylene carbonate	-3.68	-7.72	-7.80
toluene	Cc1ccccc1	propylene carbonate	-4.26	-8.52	-8.71
ethylbenzene	CCc1ccccc1	propylene carbonate	-4.82	-9.37	-9.53
isopropylbenzene	CC(C)c1ccccc1	propylene carbonate	-5.28	-9.89	-10.26
1,2-dimethylbenzene	Cc1ccccc1C	propylene carbonate	-4.75	-9.54	-9.49
1,3-dimethylbenzene	Cc1cccc(C)c1	propylene carbonate	-4.79	-9.40	-9.54
1,4-dimethylbenzene	Cc1ccc(C)cc1	propylene carbonate	-4.80	-9.29	-9.55
biphenyl	c1ccc(cc1)c2ccccc2	propylene carbonate	-8.48	-14.97	-15.20
fluorobenzene	Fc1ccccc1	propylene carbonate	-4.35	-8.36	-9.13
chlorobenzene	Clc1ccccc1	propylene carbonate	-5.33	-9.38	-10.57
bromobenzene	Brc1ccccc1	propylene carbonate	-5.59	-9.93	-10.86
iodobenzene	Ic1ccccc1	propylene carbonate	-6.60	-11.03	-12.19
nitrobenzene	[O-][N+](=O)c1ccccc1	propylene carbonate	-7.07	-12.88	-12.91
dichloromethane	ClCCl	propylene carbonate	-2.93	-6.60	-6.84
chloroform	ClC(Cl)Cl	propylene carbonate	-3.86	-7.69	-8.54
1,2-dichloroethane	ClCCCl	propylene carbonate	-3.98	-7.76	-8.35
trans-1,2-dichloroethylene	Cl/C=C/Cl	propylene carbonate	-3.82	-6.93	-8.38
trichloroethylene	ClC=C(Cl)Cl	propylene carbonate	-4.20	-8.07	-9.18
tetrachloroethylene	ClC(Cl)=C(Cl)Cl	propylene carbonate	-4.27	-8.73	-9.45
carbon dioxide	O=C=O	propylene carbonate	-0.57	-3.75	-3.84
nitromethane	C[N+](=O)[O-]	propylene carbonate	-4.38	-9.24	-9.33
sulfur dioxide	O=S=O	propylene carbonate	-3.17	-7.50	-8.89
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	propylene carbonate	-7.17	-12.50	-12.49
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	propylene carbonate	-7.81	-14.60	-14.61
water	O	propylene carbonate	-4.11	-8.55	-11.58
tetramethylstannane	C[Sn](C)(C)C	propylene carbonate	-2.38	-5.69	-5.04
imidazole	[nH]1ccnc1	propylene carbonate	-7.78	-15.34	-14.42
methane	C	carbon tetrachloride	0.22	-0.72	-0.79
ethane	CC	carbon tetrachloride	-0.73	-2.20	-2.30
propane	CCC	carbon tetrachloride	-1.54	-3.44	-3.58
butane	CCCC	carbon tetrachloride	-2.32	-4.42	-4.82
pentane	CCCCC	carbon tetrachloride	-3.11	-6.02	-6.07
hexane	CCCCCC	carbon tetrachloride	-3.83	-7.11	-7.21
heptane	CCCCCCC	carbon tetrachloride	-4.55	-8.24	-8.35
octane	CCCCCCCC	carbon tetrachloride	-5.28	-9.35	-9.56
nonane	CCCCCCCCC	carbon tetrachloride	-5.97	-10.32	-10.60
dodecane	CCCCCCCCCCC	carbon tetrachloride	-8.06	-13.79	-13.94
hexadecane	CCCCCCCCCCCCCCC	carbon tetrachloride	-10.90	-18.24	-18.43
isobutane	CC(C)C	carbon tetrachloride	-2.23	-3.86	-4.66
2,2-dimethylbutane	CCC(C)(C)C	carbon tetrachloride	-3.57	-6.19	-6.97
3-ethylpentane	CCC(CC)CC	carbon tetrachloride	-4.37	-8.10	-8.05
2,2,4,4-tetramethylpentane	CC(C)(C)CC(C)(C)C	carbon tetrachloride	-5.09	-8.66	-9.36
cyclohexane	C1CCCCC1	carbon tetrachloride	-4.26	-7.73	-7.72
cycloheptane	C1CCCCC1C	carbon tetrachloride	-4.97	-9.06	-8.83
cyclooctane	C1CCCCCCC1	carbon tetrachloride	-5.64	-10.27	-9.90
cyclodecane	C1CCCCCCCCC1	carbon tetrachloride	-6.93	-12.43	-11.98
methylcyclopentane	CC1CCCC1	carbon tetrachloride	-4.17	-7.40	-7.58
methylcyclohexane	CC1CCCCC1	carbon tetrachloride	-4.85	-8.28	-8.62
cis-decalin	C1CC[C@@H]2CCCC[C@H]2C1	carbon tetrachloride	-7.16	-12.14	-11.97
trans-decalin	C1CC[C@H]2CCCC[C@H]2C1	carbon tetrachloride	-7.11	-11.76	-11.87
bicyclohexyl	C1CCC(CC1)C2CCCCC2	carbon tetrachloride	-8.64	-13.66	-14.36
tetralin	C1CCc2ccccc2C1	carbon tetrachloride	-7.20	-13.26	-12.25
1-octene	CCCCCCC=C	carbon tetrachloride	-5.28	-9.46	-9.47
norbornadiene	C1CC2=CC=C1C2	carbon tetrachloride	-5.02	-8.49	-8.74
acetone	CC(C)=O	carbon tetrachloride	-3.13	-6.73	-6.12
methyl ethyl ketone	CCC(C)=O	carbon tetrachloride	-3.99	-7.92	-7.52
2-pentanone	CCCC(C)=O	carbon tetrachloride	-4.69	-8.86	-8.64
3-pentanone	CCC(=O)CC	carbon tetrachloride	-4.75	-9.02	-8.75
2-hexanone	CCCC(C)=O	carbon tetrachloride	-5.41	-10.00	-9.78
4-heptanone	CCCC(=O)CCC	carbon tetrachloride	-6.15	-10.91	-11.00

1-chlorobutane	CCCCCl	carbon tetrachloride	-4.09	-7.93	-7.62
1-chlorooctane	CCCCCCCCl	carbon tetrachloride	-6.98	-12.81	-12.21
trans-1,2-dichloroethylene	ClC=C\Cl	carbon tetrachloride	-3.57	-6.70	-6.68
tetrachloroethylene	ClC(Cl)=C(Cl)Cl	carbon tetrachloride	-4.81	-9.40	-8.70
1-iodobutane	CCCCI	carbon tetrachloride	-5.46	-9.65	-9.36
2-iodo-2-methylpropane	CC(C)(C)I	carbon tetrachloride	-4.95	-8.50	-8.41
diiodomethane	ICI	carbon tetrachloride	-6.34	-10.01	-10.25
chlorotrifluoromethane	FC(F)(F)Cl	carbon tetrachloride	-0.35	-2.54	-2.26
propanal	CCC=O	carbon tetrachloride	-3.27	-6.88	-6.36
butanal	CCCC=O	carbon tetrachloride	-3.98	-7.86	-7.46
pentanal	CCCCC=O	carbon tetrachloride	-4.80	-9.12	-8.81
nitromethane	C[N+](=O)[O-]	carbon tetrachloride	-3.16	-6.78	-6.38
nitroethane	CC[N+](=O)[O-]	carbon tetrachloride	-3.92	-7.86	-7.61
2-nitropropane	CC(C)[N+](=O)[O-]	carbon tetrachloride	-4.61	-8.57	-8.75
acetonitrile	CC#N	carbon tetrachloride	-3.17	-6.06	-5.50
methanol	CO	carbon tetrachloride	-1.79	-4.73	-4.18
ethanol	CCO	carbon tetrachloride	-2.58	-5.80	-5.52
1-propanol	CCCO	carbon tetrachloride	-3.36	-6.67	-6.79
isopropanol	CC(C)O	carbon tetrachloride	-3.18	-6.31	-6.54
1-butanol	CCCCO	carbon tetrachloride	-4.08	-8.25	-7.99
1-pentanol	CCCCCO	carbon tetrachloride	-4.74	-9.04	-9.04
1-hexanol	CCCCCO	carbon tetrachloride	-5.52	-10.09	-10.22
1-octanol	CCCCCCCCO	carbon tetrachloride	-6.89	-12.48	-12.43
2-methyl-2-butanol	CCC(C)(C)O	carbon tetrachloride	-4.35	-7.34	-8.64
propyl formate	CCCOC=O	carbon tetrachloride	-4.40	-8.40	-8.33
butyl formate	CCCCOC=O	carbon tetrachloride	-5.11	-9.55	-9.47
methyl acetate	COC(C)=O	carbon tetrachloride	-3.72	-7.39	-7.22
ethyl acetate	CCOC(C)=O	carbon tetrachloride	-4.28	-8.36	-8.10
methyl propionate	CCC(=O)OC	carbon tetrachloride	-4.29	-8.55	-8.10
ethyl propionate	CCOC(=O)CC	carbon tetrachloride	-4.93	-9.51	-9.11
propyl propionate	CCCOC(=O)CC	carbon tetrachloride	-5.49	-10.62	-10.00
benzene	c1ccccc1	carbon tetrachloride	-4.25	-7.96	-7.90
toluene	Cc1ccccc1	carbon tetrachloride	-4.94	-9.11	-8.96
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	carbon tetrachloride	-6.18	-11.17	-10.85
biphenyl	c1ccc(cc1)c2ccccc2	carbon tetrachloride	-8.83	-15.07	-15.04
naphthalene	c1ccc2ccccc2c1	carbon tetrachloride	-7.41	-12.94	-12.92
anthracene	c1ccc2cc3ccccc3cc2c1	carbon tetrachloride	-10.46	-18.45	-17.69
acetophenone	CC(=O)c1ccccc1	carbon tetrachloride	-6.99	-11.97	-12.16
benzaldehyde	O=Cc1ccccc1	carbon tetrachloride	-6.12	-11.20	-10.70
benzonitrile	N#Cc1ccccc1	carbon tetrachloride	-6.66	-11.50	-10.90
bromobenzene	Brc1ccccc1	carbon tetrachloride	-5.87	-10.27	-10.42
1,3-dibromobenzene	BrCc1ccc(Br)cc1	carbon tetrachloride	-7.53	-12.76	-12.98
1,4-dibromobenzene	BrCc1cc(Br)cc1	carbon tetrachloride	-7.52	-12.70	-12.96
1,3,4,5-tetrabromobenzene	BrCc1cc(Br)c(Br)c(Br)c1	carbon tetrachloride	-9.64	-16.30	-16.01
1,3-dichlorobenzene	ClCc1ccc(Cl)cc1	carbon tetrachloride	-6.50	-11.22	-11.22
1,4-dichlorobenzene	ClCc1cc(Cl)cc1	carbon tetrachloride	-6.52	-11.16	-11.24
1,2,4,5-tetrachlorobenzene	ClCc1cc(Cl)c(Cl)cc1Cl	carbon tetrachloride	-8.41	-13.88	-14.20
fluorobenzene	Fc1ccccc1	carbon tetrachloride	-4.32	-8.23	-8.05
1,2-diiodobenzene	Ic1ccccc1I	carbon tetrachloride	-8.99	-14.84	-14.10
2-bromotoluene	Cc1ccccc1Br	carbon tetrachloride	-6.46	-11.28	-11.24
3-bromotoluene	Cc1cccc(Br)c1	carbon tetrachloride	-6.48	-11.23	-11.28
4-bromotoluene	Cc1ccc(Br)cc1	carbon tetrachloride	-6.48	-11.11	-11.29
2-iodotoluene	Cc1ccccc1I	carbon tetrachloride	-7.43	-12.21	-12.26
4-iodotoluene	Cc1ccc(I)cc1	carbon tetrachloride	-7.39	-12.05	-12.21
trifluoromethylbenzene	FC(F)(F)c1ccccc1	carbon tetrachloride	-4.68	-8.21	-8.34
dimethylformamide	CN(C)C=O	carbon tetrachloride	-5.12	-10.64	-9.95
dimethyl sulfoxide	C[S](C)=O	carbon tetrachloride	-6.49	-10.75	-11.76
1-chloro-2-nitrobenzene	[O-][N+](=O)c1ccccc1Cl	carbon tetrachloride	-6.99	-13.29	-12.24
1-chloro-3-nitrobenzene	[O-][N+](=O)c1cccc(Cl)c1	carbon tetrachloride	-7.36	-13.14	-12.73
4-chloro-1-nitrobenzene	[O-][N+](=O)c1ccc(Cl)cc1	carbon tetrachloride	-7.40	-13.40	-12.80
pyrrole	[nH]1ccccc1	carbon tetrachloride	-4.94	-7.94	-9.01
N-methylpyrrole	Cn1ccccc1	carbon tetrachloride	-4.92	-9.32	-9.09
aniline	Nc1ccccc1	carbon tetrachloride	-6.15	-11.11	-10.75
N-methylaniline	CNc1ccccc1	carbon tetrachloride	-6.55	-11.85	-11.71
N,N-dimethylaniline	CN(C)c1ccccc1	carbon tetrachloride	-6.86	-12.43	-12.21
N-ethylaniline	CCNc1ccccc1	carbon tetrachloride	-7.13	-12.99	-12.71
pyridine	c1ccncc1	carbon tetrachloride	-4.89	-9.16	-8.49
2-methylpyridine	Cc1cccn1	carbon tetrachloride	-5.70	-10.28	-9.86
2,6-dimethylpyridine	Cc1cccc(C)n1	carbon tetrachloride	-6.45	-11.16	-11.16
2-bromopyridine	BrCc1cccn1	carbon tetrachloride	-6.88	-12.04	-11.71
3-bromopyridine	BrCc1cccn1	carbon tetrachloride	-6.88	-12.22	-11.66
2-chloropyridine	ClCc1cccn1	carbon tetrachloride	-6.18	-10.80	-10.55
3-cyanopyridine	N#Cc1cccn1	carbon tetrachloride	-7.28	-11.81	-11.54
4-cyanopyridine	N#Cc1ccncc1	carbon tetrachloride	-7.19	-11.74	-11.34
butylamine	CCCCN	carbon tetrachloride	-4.02	-8.49	-7.83
diethylamine	CCNCC	carbon tetrachloride	-3.96	-7.94	-8.08
tributylamine	CCCCN(CCCC)CCCC	carbon tetrachloride	-8.54	-16.42	-15.50
argon	[Ar]	carbon tetrachloride	0.58	-0.10	-0.20
nitrogen	N#N	carbon tetrachloride	0.91	0.56	0.61
carbon monoxide	C=O	carbon tetrachloride	0.62	0.30	-0.23
carbon dioxide	O=C=O	carbon tetrachloride	-0.27	-2.25	-1.81
oxygen	O=O	carbon tetrachloride	0.77	0.01	-0.03
sulfur hexafluoride	F[S](F)(F)(F)(F)F	carbon tetrachloride	-0.09	-1.67	-1.80

nitric oxide	[N]=O	carbon tetrachloride	0.33	-0.34	-0.64
tetrahydrothiophene	C1CCSC1	carbon tetrachloride	-4.84	-9.87	-7.91
diethyl sulfide	CCSCC	carbon tetrachloride	-5.06	-9.26	-8.94
dibutyl sulfide	CCCCSCCCC	carbon tetrachloride	-8.18	-13.08	-13.96
N,N-dimethylacetamide	CN(C)C(C)=O	carbon tetrachloride	-5.84	-11.37	-11.25
phenol	Oc1ccccc1	carbon tetrachloride	-5.56	-10.37	-10.00
2-chlorophenol	Oc1ccccc1Cl	carbon tetrachloride	-6.24	-11.02	-10.82
4-chlorophenol	Oc1ccc(Cl)cc1	carbon tetrachloride	-6.54	-11.59	-11.34
pentafluorophenol	Oc1c(F)c(F)c(F)c(F)c1F	carbon tetrachloride	-4.31	-10.04	-9.90
3-methylphenol	Cc1cccc(O)c1	carbon tetrachloride	-6.23	-11.01	-11.03
2,4,6-trimethylphenol	Cc1cc(C)c(O)c(C)c1	carbon tetrachloride	-7.40	-13.43	-12.98
4-tert-butylphenol	CC(C)(C)c1ccc(O)cc1	carbon tetrachloride	-8.15	-14.03	-14.29
2,4-di-tert-butylphenol	CC(C)(C)c1ccc(O)c(c1)C(C)(C)C	carbon tetrachloride	-9.99	-16.73	-17.48
2-methoxyphenol	COc1ccccc1O	carbon tetrachloride	-7.14	-13.00	-13.08
3-methoxyphenol	COc1cccc(O)c1	carbon tetrachloride	-7.49	-14.22	-13.50
4-methoxyphenol	COc1ccc(O)cc1	carbon tetrachloride	-7.55	-13.77	-13.59
γ-butyrolactone	O=C1CCCO1	carbon tetrachloride	-5.46	-11.62	-10.10
1-naphthol	Oc1ccccc2ccccc12	carbon tetrachloride	-8.54	-14.51	-14.68
phenyl methyl sulfide	CSc1ccccc1	carbon tetrachloride	-7.79	-12.62	-13.46
acrylonitrile	C=CC#N	carbon tetrachloride	-3.72	-6.50	-6.27
1,4-difluorobenzene	Fc1ccc(F)cc1	carbon tetrachloride	-4.61	-8.10	-8.62
benzophenone	O=C(c1ccccc1)c2ccccc2	carbon tetrachloride	-10.61	-17.80	-17.71
trans-stilbene	c1ccc(cc1)C=Cc2ccccc2	carbon tetrachloride	-10.26	-18.70	-17.22
quinoline	c1ccc2ncccc2c1	carbon tetrachloride	-8.42	-13.24	-14.20
1-chloronaphthalene	Clc1ccccc2ccccc12	carbon tetrachloride	-8.41	-14.91	-14.30
1-nitronaphthalene	[O-][N+](=O)c1cccc2ccccc12	carbon tetrachloride	-9.63	-15.39	-16.48
salicylaldehyde	Oc1ccccc1C=O	carbon tetrachloride	-7.13	-11.35	-12.52
tetramethylstannane	C[Sn](C)(C)C	carbon tetrachloride	-4.26	-7.57	-7.50
methane	C	toluene	0.03	-1.21	-0.78
pentane	CCCCC	toluene	-2.96	-5.95	-5.41
hexane	CCCCCC	toluene	-3.72	-6.37	-6.62
heptane	CCCCCCC	toluene	-4.49	-7.41	-7.86
octane	CCCCCCCC	toluene	-5.22	-8.48	-9.09
nonane	CCCCCCCCC	toluene	-5.95	-9.48	-10.20
decane	CCCCCCCCCC	toluene	-6.65	-10.48	-11.28
hexadecane	CCCCCCCCCCCCCCCC	toluene	-10.84	-16.75	-17.96
cyclopentane	C1CCCC1	toluene	-3.37	-6.53	-5.81
cycloheptane	C1CCCCC1	toluene	-4.89	-8.72	-8.30
cyclooctane	C1CCCCC1	toluene	-5.59	-9.84	-9.44
cis-decalin	C1CC[C@@H]2CCCC[C@H]2C1	toluene	-6.79	-11.45	-10.70
methylcyclohexane	CC1CCCCC1	toluene	-4.78	-7.94	-8.10
ethene	C=C	toluene	-0.83	-2.10	-2.04
1-hexene	CCCCC=C	toluene	-3.75	-7.03	-6.65
methyl ethyl ketone	CCC(C)=O	toluene	-4.22	-8.26	-7.63
2-pentanone	CCCC(C)=O	toluene	-4.88	-9.21	-8.65
3-pentanone	CCC(=O)CC	toluene	-4.88	-9.27	-8.64
2-heptanone	CCCCC(C)=O	toluene	-6.22	-11.44	-10.71
2-octanone	CCCCCCC(C)=O	toluene	-6.88	-12.41	-11.72
2-nonanone	CCCCCCCC(C)=O	toluene	-7.47	-13.14	-12.64
5-nonanone	CCCCC(=O)CCCC	toluene	-7.41	-12.75	-12.57
2-undecanone	CCCCCCCCC(C)=O	toluene	-8.79	-15.66	-14.69
di-tert-butylketone	CC(C)(C)C(=O)C(C)(C)C	toluene	-6.27	-10.28	-10.86
diethyl ether	CCOCC	toluene	-3.57	-6.59	-6.46
dibutyl ether	CCCCOCCCC	toluene	-6.18	-10.08	-10.56
methyl heptyl ether	CCCCCCCOC	toluene	-6.30	-10.71	-10.72
methyl tert butyl ether	COC(C)(C)C	toluene	-3.96	-6.64	-7.19
methyl tert-amyl ether	CCC(C)(C)OC	toluene	-4.53	-8.54	-8.12
tetrahydrofuran	C1CCOC1	toluene	-4.32	-8.07	-7.77
1,4-dioxane	C1COCCO1	toluene	-4.94	-9.16	-8.76
tetrahydropyran	C1CCOCC1	toluene	-4.98	-8.59	-8.78
oxirane	C1CO1	toluene	-2.95	-7.84	-5.61
tetraglyme	COCCOCCOCCOCCOC	toluene	-10.88	-19.02	-19.09
15-crown-5	C1COCCOCCOCCOCCO1	toluene	-10.70	-19.02	-19.70
18-crown-6	C1COCCOCCOCCOCCOCCO1	toluene	-13.03	-25.33	-24.09
1-fluorooctane	CCCCCCCCF	toluene	-6.20	-11.38	-10.68
1-chlorooctane	CCCCCCCCCl	toluene	-6.92	-12.04	-11.73
γ-butyrolactone	O=C1CCCO1	toluene	-5.88	-12.67	-10.66
propylamine	CCCN	toluene	-3.31	-6.90	-6.32
pentylamine	CCCCCN	toluene	-4.79	-9.08	-8.86
octylamine	CCCCCCCCN	toluene	-6.72	-12.63	-12.16
methanol	CO	toluene	-2.05	-5.54	-4.36
ethanol	CCO	toluene	-2.72	-6.67	-5.53
1-propanol	CCCO	toluene	-3.53	-7.46	-6.86
1-butanol	CCCCO	toluene	-4.28	-8.87	-8.11
1-pentanol	CCCCCO	toluene	-4.94	-10.01	-9.17
1-octanol	CCCCCCCCO	toluene	-7.15	-12.61	-12.68
isopropanol	CC(C)O	toluene	-3.32	-7.64	-6.56
2-methyl-2-butanol	CCC(C)(C)O	toluene	-4.58	-8.05	-8.85
neon	[Ne]	toluene	1.86	1.97	1.69
krypton	[Kr]	toluene	-0.01	-0.89	-0.82
xenon	[Xe]	toluene	-0.94	-1.98	-2.28
radon	[Rn]	toluene	-1.11	-3.03	-2.48



hydrogen	[H][H]	toluene	1.50	1.22	1.21
nitrogen	N#N	toluene	0.92	1.48	0.91
carbon monoxide	C=O	toluene	0.64	0.45	0.04
carbon dioxide	O=C=O	toluene	-0.56	-2.52	-2.07
oxygen	O=O	toluene	0.74	-0.14	0.19
tetrafluoromethane	FC(F)(F)F	toluene	1.15	1.43	0.50
sulfur hexafluoride	F[S](F)(F)(F)F	toluene	0.38	-1.27	-0.78
benzene	c1ccccc1	toluene	-4.41	-8.03	-7.87
toluene	Cc1ccccc1	toluene	-5.18	-9.08	-9.10
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	toluene	-6.50	-11.18	-11.14
methyl methacrylate	COC(=O)C(C)=C	toluene	-5.03	-9.23	-8.90
phenol	Oc1ccccc1	toluene	-5.99	-12.02	-10.61
2,6-dimethylphenol	Cc1cccc(C)c1O	toluene	-7.31	-12.88	-12.81
trifluoromethylbenzene	FC(c1ccccc1)(F)F	toluene	-4.51	-8.89	-7.56
propyl formate	CCCOC=O	toluene	-4.38	-8.71	-7.88
butyl formate	CCCCOC=O	toluene	-5.15	-9.71	-9.15
butyl acetate	CCCCOC(C)=O	toluene	-5.78	-10.57	-10.18
methyl propanoate	CCC(=O)OC	toluene	-4.39	-8.46	-7.88
cyclohexyl acetate	CC(=O)OC1CCCCC1	toluene	-7.68	-12.55	-13.27
ethyl benzoate	CCOC(=O)c1ccccc1	toluene	-8.12	-14.02	-13.72
1-butanethiol	CCCCS	toluene	-5.19	-8.80	-8.62
bromobenzene	Brc1ccccc1	toluene	-5.86	-10.59	-9.99
1,3-dichlorobenzene	Clc1cccc(Cl)c1	toluene	-6.84	-11.58	-11.53
chlorobenzene	Clc1ccccc1	toluene	-5.68	-9.91	-9.81
fluorobenzene	Fc1ccccc1	toluene	-4.41	-8.30	-7.87
1-nitronaphthalene	[O-][N+](=O)c1cccc2ccccc12	toluene	-9.95	-16.60	-16.88
4-chloronitrobenzene	[O-][N+](=O)c1ccc(Cl)cc1	toluene	-7.90	-13.50	-13.65
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	toluene	-6.45	-11.77	-10.79
N-methylpyrrole	Cn1ccccc1	toluene	-5.06	-9.51	-9.00
dimethylformamide	CN(C)C=O	toluene	-5.34	-11.85	-10.01
naphthalene	c1ccc2ccccc2c1	toluene	-7.76	-13.68	-13.25
water	O	toluene	-1.85	-4.25	-4.59
anthracene	c1ccc2cc3ccccc3cc2c1	toluene	-10.78	-18.67	-17.94
pentane	CCCCC	chloroform	-2.99	-5.79	-5.86
hexane	CCCCCC	chloroform	-3.70	-6.75	-6.97
heptane	CCCCCCC	chloroform	-4.40	-7.88	-8.10
octane	CCCCCCCC	chloroform	-5.04	-8.98	-9.18
nonane	CCCCCCCCC	chloroform	-5.77	-10.03	-10.30
decane	CCCCCCCCC	chloroform	-6.49	-11.02	-11.43
undecane	CCCCCCCCCCC	chloroform	-7.08	-12.25	-12.44
dodecane	CCCCCCCCCCCC	chloroform	-7.77	-13.34	-13.55
tetradecane	CCCCCCCCCCCCC	chloroform	-9.11	-15.62	-15.71
heptadecane	CCCCCCCCCCCCCCC	chloroform	-10.71	-18.66	-18.31
cyclohexane	C1CCCCC1	chloroform	-4.29	-7.24	-7.74
cycloheptane	C1CCCCC1	chloroform	-4.98	-8.60	-8.84
cyclooctane	C1CCCCC1	chloroform	-5.63	-9.75	-9.89
benzene	c1ccccc1	chloroform	-4.57	-8.57	-8.28
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	chloroform	-6.40	-12.02	-11.10
naphthalene	c1ccc2ccccc2c1	chloroform	-7.81	-13.67	-13.36
phenanthrene	c1ccc2c(c1)ccc3ccccc23	chloroform	-11.05	-18.44	-18.46
diethyl ether	CCOCC	chloroform	-3.91	-8.70	-7.38
dipentyl ether	CCCCCOCCCC	chloroform	-7.91	-13.67	-13.89
ethoxypropane	CCCOCC	chloroform	-4.52	-9.26	-8.38
ethoxybutane	CCCCOCC	chloroform	-5.15	-11.21	-9.36
methyl tert-butyl ether	COC(C)(C)C	chloroform	-3.97	-9.21	-7.54
furan	c1ccccc1	chloroform	-4.36	-6.96	-7.98
tetrahydrofuran	C1CCOC1	chloroform	-4.70	-10.18	-8.60
tetrahydropyran	C1CCOCC1	chloroform	-5.32	-10.51	-9.58
1,4-dioxane	C1COCCO1	chloroform	-5.37	-11.88	-9.64
diglyme	COCCOCCOC	chloroform	-7.37	-17.30	-12.92
12-crown-4	C1COCCOCCOCCO1	chloroform	-9.43	-21.37	-17.73
15-crown-5	C1COCCOCCOCCOCCO1	chloroform	-11.58	-25.23	-22.10
18-crown-6	C1COCCOCCOCCOCCOCCO1	chloroform	-13.42	-31.33	-25.69
acetone	CC(C)=O	chloroform	-4.01	-9.40	-7.51
3-pentanone	CCC(=O)CC	chloroform	-5.38	-11.41	-9.63
4-heptanone	CCCC(=O)CCC	chloroform	-6.76	-13.40	-11.94
cyclohexanone	O=C1CCCCC1	chloroform	-6.54	-13.36	-11.33
dimethylformamide	CN(C)C=O	chloroform	-6.17	-14.34	-11.69
dimethyl sulfoxide	C[S](C)=O	chloroform	-7.99	-15.94	-14.45
ethyl formate	CCOC=O	chloroform	-4.22	-8.37	-7.80
propyl formate	CCCOC=O	chloroform	-4.89	-10.51	-8.87
methyl acetate	COC(C)=O	chloroform	-4.46	-9.48	-8.16
ethyl acetate	CCOC(C)=O	chloroform	-4.99	-10.48	-9.06
propyl acetate	CCCOC(C)=O	chloroform	-5.63	-11.80	-10.16
propyl propanoate	CCCOC(=O)CC	chloroform	-6.16	-12.72	-11.03
ethyl butanoate	CCCC(=O)OCC	chloroform	-6.17	-12.63	-11.02
propyl butanoate	CCCOC(=O)CCC	chloroform	-6.84	-13.57	-12.15
methyl benzoate	COC(=O)c1ccccc1	chloroform	-8.15	-14.77	-13.79
ethyl benzoate	CCOC(=O)c1ccccc1	chloroform	-8.74	-15.85	-14.80
triethylamine	CCN(CC)CC	chloroform	-4.94	-11.09	-9.78
aniline	Nc1ccccc1	chloroform	-7.06	-13.41	-12.05
N-methylaniline	CNc1ccccc1	chloroform	-7.59	-13.57	-13.48
N,N-dimethylaniline	CN(C)c1ccccc1	chloroform	-7.60	-13.92	-13.50

N-ethylaniline	CCNc1ccccc1	chloroform	-8.12	-14.53	-14.51
pyridine	c1ccncc1	chloroform	-5.95	-11.57	-10.05
2-methylpyridine	Cc1cccn1	chloroform	-6.84	-12.67	-11.64
4-methylpyridine	Cc1ccncc1	chloroform	-6.82	-13.36	-11.54
acetonitrile	CC#N	chloroform	-4.51	-8.83	-7.50
ethanol	CCO	chloroform	-3.48	-7.84	-7.20
1-propanol	CCCO	chloroform	-4.27	-8.41	-8.52
isopropanol	CC(C)O	chloroform	-3.97	-8.39	-8.06
1-butanol	CCCCO	chloroform	-4.93	-10.04	-9.64
1-octanol	CCCCCCCCO	chloroform	-7.57	-14.34	-13.80
dichloromethane	ClCCl	chloroform	-3.27	-7.25	-6.11
chloroform	ClC(Cl)Cl	chloroform	-4.05	-7.48	-7.34
1-chlorobutane	CCCCCl	chloroform	-4.39	-8.38	-8.14
1,2-dichloroethane	ClCCCl	chloroform	-4.41	-8.52	-7.90
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	chloroform	-6.41	-10.91	-10.86
phenol	Oc1ccccc1	chloroform	-6.70	-12.19	-11.89
2-methoxyphenol	COc1ccccc1O	chloroform	-8.54	-14.81	-15.61
anisole	COc1ccccc1	chloroform	-6.46	-12.06	-11.14
pyrrole	[nH]1ccccc1	chloroform	-5.90	-9.83	-10.44
N-methylpyrrole	Cn1ccccc1	chloroform	-5.59	-11.17	-10.16
diethyl sulfide	CCSCC	chloroform	-5.60	-10.40	-10.04
piperidine	C1CCNCC1	chloroform	-6.20	-11.83	-11.60
nitrobenzene	[O-][N+](=O)c1ccccc1	chloroform	-7.50	-14.15	-12.88
bromoethane	CCBr	chloroform	-3.40	-6.67	-6.65
1,2-diaminobenzene	Nc1ccccc1N	chloroform	-8.07	-14.67	-15.20
1-chloropentane	CCCCC1	chloroform	-5.14	-9.60	-9.37
1-chlorohexane	CCCCCC1	chloroform	-5.86	-10.62	-10.49
methyl propanoate	CCC(=O)OC	chloroform	-4.91	-10.77	-8.87
methyl butanoate	CCCC(=O)OC	chloroform	-5.66	-12.05	-10.14
methyl pentanoate	CCCCC(=O)OC	chloroform	-6.28	-12.57	-11.16
methyl hexanoate	CCCCCC(=O)OC	chloroform	-6.95	-13.85	-12.23
methyl octanoate	CCCCCCCC(=O)OC	chloroform	-8.18	-16.10	-14.28
methyl nonanoate	CCCCCCCCC(=O)OC	chloroform	-8.73	-16.96	-15.20
methyl decanoate	CCCCCCCCC(=O)OC	chloroform	-9.74	-18.10	-16.78
anthracene	c1ccc2cc3ccccc3cc2c1	chloroform	-11.06	-19.62	-18.45
tetramethylstannane	C[Sn](C)(C)C	chloroform	-4.21	-7.15	-7.27
N-methylimidazole	Cn1ccnc1	chloroform	-7.61	-15.30	-13.14
pentane	CCCCC	tert-butanol	-2.97	-5.45	-6.04
hexane	CCCCCC	tert-butanol	-3.69	-6.62	-7.19
heptane	CCCCCCC	tert-butanol	-4.41	-7.53	-8.39
dodecane	CCCCCCCCCCCC	tert-butanol	-7.76	-12.78	-13.82
tetradecane	CCCCCCCCCCCCC	tert-butanol	-9.00	-15.18	-15.79
hexadecane	CCCCCCCCCCCCCCC	tert-butanol	-10.20	-16.87	-17.60
3-ethylpentane	CCC(CC)CC	tert-butanol	-4.16	-7.29	-8.01
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	tert-butanol	-4.24	-7.37	-8.18
cyclohexane	C1CCCCC1	tert-butanol	-3.91	-6.87	-6.98
cis-2-butene	C/C=C/C	tert-butanol	-2.40	-4.31	-4.93
aniline	Nc1ccccc1	tert-butanol	-7.65	-10.65	-13.48
toluene	Cc1ccccc1	tert-butanol	-4.84	-7.32	-8.46
1,3-dimethylbenzene	Cc1ccc(C)c1	tert-butanol	-5.43	-9.27	-9.37
naphthalene	c1ccc2ccccc2c1	tert-butanol	-7.44	-10.83	-12.49
biphenyl	c1ccc(cc1)c2ccccc2	tert-butanol	-8.98	-12.49	-14.72
trifluorotoluene	FC(F)(F)c1ccccc1	tert-butanol	-5.01	-6.90	-8.72
nitrobenzene	[O-][N+](=O)c1ccccc1	tert-butanol	-7.28	-9.31	-12.52
anisole	COc1ccccc1	tert-butanol	-5.93	-8.33	-9.97
3-methylphenol	Cc1ccc(O)c1	tert-butanol	-8.66	-15.79	-16.10
1-butanol	CCCCO	tert-butanol	-5.80	-13.01	-11.83
1-pentanol	CCCCCO	tert-butanol	-6.30	-14.11	-12.55
1-decanol	CCCCCCCCCO	tert-butanol	-9.37	-19.43	-17.50
2-methyl-2-butanol	CCC(C)(C)O	tert-butanol	-5.08	-11.88	-10.48
2-methyl-isopropanol	CC(C)(C)O	tert-butanol	-4.61	-11.19	-9.69
butane-1,4-diol	OCCCCO	tert-butanol	-8.79	-20.12	-18.08
diethyl ether	CCOCC	tert-butanol	-3.37	-5.96	-6.18
methyl butyl ether	CCCCOC	tert-butanol	-4.10	-7.05	-7.40
methyl tert-butyl ether	COC(C)(C)C	tert-butanol	-3.35	-7.03	-6.22
2-methyltetrahydrofuran	CC1CCCO1	tert-butanol	-4.06	-7.76	-6.85
1,3-dioxolane	C1COCO1	tert-butanol	-3.66	-6.54	-6.36
1,4-dioxane	C1COCCO1	tert-butanol	-4.52	-7.27	-7.63
acetone	CC(C)=O	tert-butanol	-3.38	-5.79	-6.14
butanone	CCC(C)=O	tert-butanol	-4.18	-6.74	-7.42
2-heptanone	CCCCCC(C)=O	tert-butanol	-6.12	-9.97	-10.45
4-heptanone	CCCC(=O)CCC	tert-butanol	-6.18	-9.72	-10.60
2-nonanone	CCCCCCCC(C)=O	tert-butanol	-7.55	-12.16	-12.86
cyclohexanone	O=C1CCCCC1	tert-butanol	-6.36	-9.82	-10.99
chloroethane	CCCl	tert-butanol	-2.59	-5.24	-5.13
butyl formate	CCCCOC=O	tert-butanol	-4.90	-7.77	-8.46
ethyl acetate	CCOC(C)=O	tert-butanol	-4.01	-6.77	-6.89
butyl acetate	CCCCOC(C)=O	tert-butanol	-5.22	-8.88	-8.90
methyl propanoate	CCC(=O)OC	tert-butanol	-3.98	-6.89	-6.79
ethyl propanoate	CCOC(=O)CC	tert-butanol	-4.61	-7.82	-7.88
butyl propanoate	CCCCOC(=O)CC	tert-butanol	-5.97	-9.96	-10.26
methyl butanoate	CCCC(=O)OC	tert-butanol	-4.73	-7.78	-8.05
propyl butanoate	CCCOC(=O)CCC	tert-butanol	-6.03	-9.83	-10.36

dimethyl carbonate	COC(=O)OC	tert-butanol	-4.13	-5.96	-7.02
diethyl carbonate	CCOC(=O)OCC	tert-butanol	-4.95	-7.82	-8.44
1-butanenitrile	CCCC#N	tert-butanol	-5.28	-7.01	-8.33
1-chlorobutane	CCCCCl	tert-butanol	-3.88	-6.30	-7.10
2-chlorobutane	CCC(C)Cl	tert-butanol	-3.73	-6.04	-6.83
2-methyl-1-chlorobutane	CCC(C)CCl	tert-butanol	-4.33	-6.10	-7.79
2-chloro-2-methylpropane	CC(C)(C)Cl	tert-butanol	-3.35	-5.42	-6.22
tetrachloromethane	ClC(Cl)(Cl)Cl	tert-butanol	-4.38	-6.66	-8.15
2-methyl-2-bromopropane	CC(C)(C)Br	tert-butanol	-3.69	-5.87	-6.84
2-methyl-2-iodopropane	CC(C)(C)I	tert-butanol	-4.29	-6.66	-7.13
tetramethylsilane	C[Si](C)(C)C	tert-butanol	-3.01	-4.83	-5.43
chlorobenzene	Clc1ccccc1	tert-butanol	-5.44	-7.77	-9.30
bromobenzene	Brc1ccccc1	tert-butanol	-5.73	-8.43	-9.76
iodobenzene	Ic1ccccc1	tert-butanol	-6.36	-9.47	-10.11
nitromethane	C[N+](=[O-])=O	tert-butanol	-4.22	-5.64	-8.01
β-pinene	CC1(C)C2CCC(=C)C1C2	tert-butanol	-6.27	-9.89	-10.45
methyl tert-amyl ether	CCC(C)(C)OC	tert-butanol	-3.96	-8.15	-7.27
adipic acid	OC(=O)CCCCC(O)=O	tert-butanol	-12.52	-27.39	-24.97
1-bromoadamantane	BrC12CC3CC(CC(C3)C1)C2	tert-butanol	-8.05	-12.44	-12.82
ethylene carbonate	O=C1OCCO1	tert-butanol	-5.40	-7.39	-9.54
2-pyrrolidone	O=C1CCCN1	tert-butanol	-8.59	-15.79	-15.81
hydrogen sulfide	S	tert-butanol	-1.74	-2.54	-2.82
hexane	CCCCCC	2-methyl-2-butanol	-3.81	-7.04	-7.41
nonane	CCCCCCCCC	2-methyl-2-butanol	-6.00	-10.38	-11.02
dodecane	CCCCCCCCCCCC	2-methyl-2-butanol	-8.11	-13.62	-14.51
hexadecane	CCCCCCCCCCCCCCCC	2-methyl-2-butanol	-10.73	-18.11	-18.62
3-ethylpentane	CCC(CC)CC	2-methyl-2-butanol	-4.40	-7.90	-8.46
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	2-methyl-2-butanol	-4.31	-7.91	-8.26
cyclohexane	C1CCCCC1	2-methyl-2-butanol	-4.01	-7.40	-7.19
cyclooctane	C1CCCCCCC1	2-methyl-2-butanol	-5.47	-9.75	-9.62
bicyclohexyl	C1CCC(CC1)C2CCCCC2	2-methyl-2-butanol	-7.90	-13.15	-12.79
1-heptene	CCCCCC=C	2-methyl-2-butanol	-4.72	-7.94	-8.79
benzene	c1ccccc1	2-methyl-2-butanol	-4.27	-6.84	-7.71
tetrachloromethane	ClC(Cl)(Cl)Cl	2-methyl-2-butanol	-4.46	-7.26	-8.34
methyl tert-amyl ether	CCC(C)(C)OC	2-methyl-2-butanol	-3.97	-8.36	-7.32
dibutylamine	CCCCNCCCC	2-methyl-2-butanol	-6.46	-13.29	-13.12
triethylamine	CCN(CC)CC	2-methyl-2-butanol	-4.55	-8.98	-9.08
tripropylamine	CCCN(CCC)CCC	2-methyl-2-butanol	-6.20	-10.64	-12.05
pentane	CCCCC	diethyl ether	-3.36	-6.04	-6.56
hexane	CCCCCC	diethyl ether	-4.06	-7.15	-7.65
heptane	CCCCCCC	diethyl ether	-4.74	-8.34	-8.71
decane	CCCCCCCCC	diethyl ether	-6.79	-11.76	-11.91
dodecane	CCCCCCCCCCCC	diethyl ether	-8.05	-13.99	-13.82
hexadecane	CCCCCCCCCCCCCCCC	diethyl ether	-10.65	-18.60	-17.83
2-methylpentane	CCCC(C)C	diethyl ether	-3.94	-6.89	-7.48
cyclohexane	C1CCCCC1	diethyl ether	-4.21	-7.48	-7.43
ethanol	CCO	diethyl ether	-4.33	-8.86	-9.23
1-propanol	CCCO	diethyl ether	-5.00	-10.09	-10.27
1-butanol	CCCCO	diethyl ether	-5.54	-11.24	-11.06
nitromethane	C[N+](=[O-])=O	diethyl ether	-3.92	-8.73	-7.81
nitroethane	CC[N+](=[O-])=O	diethyl ether	-4.61	-9.22	-8.82
acetonitrile	CC#N	diethyl ether	-3.94	-7.35	-6.46
propionitrile	CCC#N	diethyl ether	-4.63	-8.18	-7.53
1-chloropropane	CCCCl	diethyl ether	-3.67	-6.96	-7.10
chloroform	ClC(Cl)Cl	diethyl ether	-4.63	-9.38	-8.67
tetrachloromethane	ClC(Cl)(Cl)Cl	diethyl ether	-4.96	-8.21	-9.05
diethyl ether	CCOCC	diethyl ether	-3.66	-6.48	-6.79
formamide	NC=O	diethyl ether	-6.39	-13.67	-12.94
methylformamide	CNC=O	diethyl ether	-6.40	-11.62	-12.44
dimethylformamide	CN(C)C=O	diethyl ether	-5.82	-9.99	-10.87
chlorobenzene	Clc1ccccc1	diethyl ether	-6.01	-10.23	-10.66
triethylamine	CCN(CC)CC	diethyl ether	-4.56	-8.10	-8.15
benzene	c1ccccc1	diethyl ether	-4.81	-8.11	-8.77
toluene	Cc1ccccc1	diethyl ether	-5.38	-9.19	-9.64
bromobenzene	Brc1ccccc1	diethyl ether	-6.30	-11.02	-11.10
nitrobenzene	[O-][N+](=O)c1ccccc1	diethyl ether	-7.26	-13.13	-12.86
1,4-dibromobenzene	Brc1ccc(Br)cc1	diethyl ether	-7.71	-13.19	-13.21
4-nitrotoluene	Cc1ccc(cc1)[N+](=[O-])=O	diethyl ether	-8.02	-14.40	-14.06
1,4-dinitrobenzene	[O-][N+](=O)c1ccc(cc1)[N+](=[O-])=O	diethyl ether	-9.37	-16.44	-16.73
1,3-dinitrobenzene	[O-][N+](=O)c1cccc(c1)[N+](=[O-])=O	diethyl ether	-9.36	-16.09	-16.74
N,N-dimethylaniline	CN(C)c1ccccc1	diethyl ether	-6.96	-12.41	-11.72
benzaldehyde	O=Cc1ccccc1	diethyl ether	-6.92	-11.51	-11.95
N,N-dimethyl-3-nitroaniline	CN(C)c1ccc(cc1)[N+](=[O-])=O	diethyl ether	-9.13	-16.66	-15.62
N,N-dimethyl-4-nitroaniline	CN(C)c1ccc(cc1)[N+](=[O-])=O	diethyl ether	-9.04	-16.95	-15.40
1,4-dimethylbenzene	Cc1ccc(C)cc1	diethyl ether	-5.94	-10.22	-10.50
4-(N,N-dimethylamino)nitrosobenzene	CN(C)c1ccc(cc1)N=O	diethyl ether	-9.35	-13.90	-15.86
pentane	CCCCC	dibutyl ether	-3.15	-6.28	-6.52
heptane	CCCCCCC	dibutyl ether	-4.65	-8.62	-8.90
octane	CCCCCCCC	dibutyl ether	-5.24	-9.79	-9.76
nonane	CCCCCCCCC	dibutyl ether	-6.04	-10.93	-11.07

dodecane	CCCCCCCCCCCC	dibutyl ether		-8.04	-14.37	-14.17
hexadecane	CCCCCCCCCCCCCCCC	dibutyl ether		-10.84	-19.02	-18.64
3-ethylpentane	CCC(CC)CC	dibutyl ether		-4.47	-8.34	-8.59
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	dibutyl ether		-4.45	-8.32	-8.45
methylcyclohexane	CC1CCCCC1	dibutyl ether		-4.69	-8.39	-8.55
1-hexene	CCCCC=C	dibutyl ether		-3.97	-7.34	-7.74
1-octene	CCCCCCC=C	dibutyl ether		-5.44	-9.66	-10.05
4-octyne	CCCC#CCCC	dibutyl ether		-5.23	-10.28	-9.46
ethylbenzene	CCc1ccccc1	dibutyl ether		-5.67	-10.04	-10.24
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	dibutyl ether		-6.07	-10.37	-10.82
methanol	CO	dibutyl ether		-2.96	-7.47	-7.31
ethanol	CCO	dibutyl ether		-3.65	-8.44	-8.42
propan-1-ol	CCCO	dibutyl ether		-4.39	-9.43	-9.59
propan-2-ol	CC(C)O	dibutyl ether		-4.12	-9.47	-9.07
butan-1-ol	CCCCO	dibutyl ether		-4.91	-10.74	-10.30
butan-2-ol	CCC(C)O	dibutyl ether		-4.80	-9.72	-10.17
2-methylpropan-1-ol	CC(C)CO	dibutyl ether		-4.75	-10.65	-10.03
tert-butanol	CC(C)(C)O	dibutyl ether		-4.05	-8.87	-8.82
pentan-1-ol	CCCCCO	dibutyl ether		-5.72	-11.64	-11.64
2-pentanol	CCCC(C)O	dibutyl ether		-5.31	-10.81	-10.85
3-pentanol	CCC(O)CC	dibutyl ether		-5.36	-10.50	-10.98
3-methyl-2-butanol	CC(C)C(C)O	dibutyl ether		-5.04	-9.79	-10.42
2,2-dimethylpropan-1-ol	CC(C)(C)CO	dibutyl ether		-4.73	-9.71	-9.88
heptan-1-ol	CCCCCCCO	dibutyl ether		-6.96	-14.11	-13.51
2-methylbutan-2-ol	CCC(C)(C)O	dibutyl ether		-4.57	-9.27	-9.56
2-butoxyethanol	CCCCOCCO	dibutyl ether		-6.67	-12.13	-12.96
dipropyl ether	CCCOCC	dibutyl ether		-4.80	-7.66	-8.97
butyl methyl ether	CCCCOC	dibutyl ether		-4.13	-7.72	-7.90
methyl tert-butyl ether	COC(C)(C)C	dibutyl ether		-3.38	-6.93	-6.62
tetrahydrofuran	C1CCOC1	dibutyl ether		-3.92	-7.42	-7.45
acetone	CC(C)=O	dibutyl ether		-2.89	-6.22	-5.85
butanone	CCC(C)=O	dibutyl ether		-3.70	-7.35	-7.13
pentan-2-one	CCCC(C)=O	dibutyl ether		-4.35	-8.39	-8.15
pentan-3-one	CCC(=O)CC	dibutyl ether		-4.42	-8.57	-8.25
hexan-2-one	CCCCC(C)=O	dibutyl ether		-5.08	-9.56	-9.29
heptan-2-one	CCCCCC(C)=O	dibutyl ether		-5.63	-10.59	-10.10
heptan-4-one	CCCC(=O)CCC	dibutyl ether		-5.71	-10.62	-10.27
octan-2-one	CCCCCCC(C)=O	dibutyl ether		-6.36	-11.79	-11.24
di-tert-butylketone	CC(C)(C)C(=O)C(C)(C)C	dibutyl ether		-5.73	-10.59	-10.29
cyclopentanone	O=C1CCCC1	dibutyl ether		-5.34	-9.29	-10.07
cyclohexanone	O=C1CCCCC1	dibutyl ether		-5.95	-9.94	-10.92
propylamine	CCCN	dibutyl ether		-3.74	-6.75	-7.85
diethylamine	CCNCC	dibutyl ether		-4.02	-7.29	-8.45
dibutylamine	CCCNCCCC	dibutyl ether		-6.24	-11.77	-12.35
1-chloropentane	CCCCCl	dibutyl ether		-4.71	-9.12	-8.87
1-bromobutane	CCCCBr	dibutyl ether		-4.39	-8.69	-8.44
nitrobenzene	[O-][N+](=O)c1ccccc1	dibutyl ether		-6.34	-12.18	-11.51
anisole	COc1ccccc1	dibutyl ether		-5.88	-10.64	-10.59
N,N-dimethylaniline	CN(C)c1ccccc1	dibutyl ether		-6.69	-12.10	-11.86
methyl methacrylate	COC(=O)C(C)=C	dibutyl ether		-4.36	-8.76	-8.04
3-methylphenol	Cc1cccc(O)c1	dibutyl ether		-7.56	-16.02	-14.46
trifluoromethylbenzene	FC(F)(F)c1ccccc1	dibutyl ether		-4.96	-8.95	-9.17
hexafluorobenzene	Fc1c(F)c(F)c(F)c(F)c1F	dibutyl ether		-3.38	-7.98	-8.09
benzyl alcohol	OCc1ccccc1	dibutyl ether		-7.74	-13.89	-14.75
chloroform	ClC(Cl)Cl	dibutyl ether		-4.08	-9.03	-7.89
acetic acid	CC(O)=O	dibutyl ether		-4.65	-11.98	-10.14
propanoic acid	CCC(O)=O	dibutyl ether		-5.39	-12.90	-11.43
butanoic acid	CCCC(O)=O	dibutyl ether		-5.98	-13.64	-12.38
hexanoic acid	CCCCCC(O)=O	dibutyl ether		-7.04	-16.57	-13.94
pentane	CCCCC	ethyl acetate		-2.81	-5.09	-5.42
hexane	CCCCCC	ethyl acetate		-3.48	-6.14	-6.45
decane	CCCCCCCCC	ethyl acetate		-6.07	-10.00	-10.36
undecane	CCCCCCCCCCC	ethyl acetate		-6.62	-11.47	-11.17
dodecane	CCCCCCCCCCCC	ethyl acetate		-7.25	-11.96	-12.10
pentadecane	CCCCCCCCCCCCC	ethyl acetate		-9.22	-15.21	-15.17
heptadecane	CCCCCCCCCCCCCCC	ethyl acetate		-10.30	-17.63	-16.74
2-methylpentane	CCCC(C)C	ethyl acetate		-3.30	-5.70	-6.13
3-methylpentane	CCC(C)CC	ethyl acetate		-3.29	-5.89	-6.11
3-methylhexane	CCCC(C)CC	ethyl acetate		-3.92	-6.98	-7.05
3-ethylpentane	CCC(CC)CC	ethyl acetate		-3.93	-6.95	-7.09
methyl ethyl ketone	CCC(C)=O	ethyl acetate		-4.41	-8.19	-8.26
2-pentanone	CCCC(C)=O	ethyl acetate		-5.09	-9.03	-9.35
2-hexanone	CCCCC(C)=O	ethyl acetate		-5.67	-9.93	-10.18
2-heptanone	CCCCCC(C)=O	ethyl acetate		-6.26	-10.98	-11.04
2-octanone	CCCCCCC(C)=O	ethyl acetate		-6.93	-11.77	-12.07
2-nonanone	CCCCCCCC(C)=O	ethyl acetate		-7.52	-12.91	-12.97
5-nonanone	CCCCC(=O)CCCC	ethyl acetate		-7.39	-12.36	-12.72
cyclohexanone	O=C1CCCCC1	ethyl acetate		-6.26	-10.52	-11.00
methanol	CO	ethyl acetate		-3.49	-7.62	-7.98
ethanol	CCO	ethyl acetate		-4.14	-8.46	-9.04
1-propanol	CCCO	ethyl acetate		-4.86	-9.28	-10.17
1-pentanol	CCCCCO	ethyl acetate		-5.87	-11.34	-11.53
1-octanol	CCCCCCCCO	ethyl acetate		-7.97	-14.26	-14.80

isopropanol	CC(C)O	ethyl acetate	-4.49	-8.88	-9.52
3-methyl-1-butanol	CC(C)CCO	ethyl acetate	-6.02	-10.89	-11.86
diethyl ether	CCOCC	ethyl acetate	-3.46	-6.21	-6.43
dibutyl ether	CCCCOCCCC	ethyl acetate	-5.94	-9.75	-10.19
methyl <i>tert</i> -butyl ether	COC(C)(C)C	ethyl acetate	-3.37	-7.02	-6.18
methyl heptyl ether	CCCCCCCOC	ethyl acetate	-6.17	-10.36	-10.56
2,5-dioxahexane	COCCOC	ethyl acetate	-4.66	-8.60	-8.27
2,5,8-trioxanonane	COCCOCCOC	ethyl acetate	-6.75	-11.16	-11.65
2,5,8,11-tetraoxadodecane	COCCOCCOCCOC	ethyl acetate	-8.75	-15.01	-14.76
2,5,8,11,14-pentaoxapentadecane	COCCOCCOCCOCCOC	ethyl acetate	-10.38	-18.24	-17.39
12-crown-4	C1COCCOCCOCCO1	ethyl acetate	-8.17	-15.61	-14.27
15-crown-5	C1COCCOCCOCCOCCO1	ethyl acetate	-10.02	-18.96	-17.96
chloroform	ClC(Cl)Cl	ethyl acetate	-4.10	-8.82	-7.52
2-chloro-2-methylpropane	CC(C)(C)Cl	ethyl acetate	-3.69	-6.69	-7.05
1-chlorobutane	CCCCl	ethyl acetate	-4.08	-7.69	-7.65
1-chlorooctane	CCCCCCCCCl	ethyl acetate	-6.67	-11.71	-11.58
1-chlorononane	CCCCCCCCCl	ethyl acetate	-7.40	-12.47	-12.78
trichloroethene	ClC=C(Cl)Cl	ethyl acetate	-4.69	-8.78	-8.65
2-bromo-2-methylpropane	CC(C)(C)Br	ethyl acetate	-4.09	-7.34	-7.82
1,2-dibromoethane	BrCCBr	ethyl acetate	-5.55	-9.87	-10.05
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	ethyl acetate	-6.05	-10.83	-10.37
naphthalene	c1ccc2ccccc2c1	ethyl acetate	-7.57	-13.36	-12.86
biphenyl	c1ccc(cc1)c2ccccc2	ethyl acetate	-9.17	-15.39	-15.31
anthracene	c1ccc2cc3ccccc3cc2c1	ethyl acetate	-10.81	-18.31	-17.98
2,2,2-trifluoroethanol	OCC(F)(F)F	ethyl acetate	-4.67	-10.99	-11.65
ethyl acetate	CCOC(C)=O	ethyl acetate	-4.59	-8.40	-8.60
3-methylphenol	Cc1cccc(O)c1	ethyl acetate	-8.48	-16.08	-15.97
(trifluoromethyl)benzene	FC(F)(F)c1ccccc1	ethyl acetate	-5.39	-9.01	-9.51
nitrobenzene	[O-][N+](=O)c1ccccc1	ethyl acetate	-7.25	-13.39	-12.90
anisole	COc1ccccc1	ethyl acetate	-6.40	-11.26	-11.19
nitric oxide	[N]=O	ethyl acetate	-0.26	-0.60	-1.84
pyrrole	[nH]1ccccc1	ethyl acetate	-6.26	-11.84	-11.46
<i>N</i> -methylpyrrole	Cn1ccccc1	ethyl acetate	-5.37	-9.67	-9.50
triethylamine	CCN(CC)CC	ethyl acetate	-4.14	-7.60	-7.47
1-bromoadamantane	BrC12CC3CC(C(C3)C1)C2	ethyl acetate	-8.25	-13.34	-13.21
1-adamantanol	OC12CC3CC(C(C3)C1)C2	ethyl acetate	-9.60	-15.25	-16.58
salicylamide	NC(=O)c1ccccc1O	ethyl acetate	-10.73	-19.96	-19.32
phenol	Oc1ccccc1	ethyl acetate	-7.94	-15.40	-15.18
benzaldehyde	O=Cc1ccccc1	ethyl acetate	-7.23	-12.10	-12.79
pyridine	c1ccncc1	ethyl acetate	-5.79	-9.53	-9.68
aniline	Nc1ccccc1	ethyl acetate	-8.02	-14.17	-14.64
2-methylpyridine	Cc1cccn1	ethyl acetate	-6.44	-10.16	-10.79
1-butylamine	NCCCC	ethyl acetate	-5.38	-8.33	-10.71
acetic acid	CC(O)=O	ethyl acetate	-5.91	-11.34	-12.55
formic acid	OC=O	ethyl acetate	-5.40	-11.60	-11.90
formamide	NC=O	ethyl acetate	-6.67	-13.72	-13.38
methylformamide	CNC=O	ethyl acetate	-6.70	-11.90	-12.85
dimethylformamide	CN(C)C=O	ethyl acetate	-6.08	-11.07	-11.36
acetamide	CC(N)=O	ethyl acetate	-7.25	-14.17	-14.20
<i>N</i> -methylacetamide	CNC(C)=O	ethyl acetate	-7.33	-15.24	-14.02
2-pyrrolidone	O=C1CCCN1	ethyl acetate	-8.27	-15.10	-15.18
$\gamma$ -butyrolactam	O=C1CCCN1	ethyl acetate	-8.27	-16.20	-15.18
<i>N</i> -methylbutyrolactam	CN1CCCC1=O	ethyl acetate	-7.71	-13.72	-13.79
$\delta$ -valerolactam	O=C1CCCCN1	ethyl acetate	-8.60	-15.27	-15.60
<i>N</i> -methylvalerolactam	CN1CCCC1=O	ethyl acetate	-8.15	-13.77	-14.44
$\epsilon$ -caprolactam	O=C1CCCCCN1	ethyl acetate	-8.99	-16.01	-16.21
<i>N</i> -methylcaprolactam	CN1CCCCC1=O	ethyl acetate	-8.52	-14.67	-14.96
tetramethylstannane	C[Sn](C)(C)C	ethyl acetate	-3.98	-6.49	-6.38
neon	[Ne]	dimethyl carbonate	2.23	3.66	2.46
argon	[Ar]	dimethyl carbonate	1.20	1.82	0.78
krypton	[Kr]	dimethyl carbonate	0.43	-0.60	-0.26
xenon	[Xe]	dimethyl carbonate	-0.25	-1.35	-1.18
sulfur hexafluoride	F[S](F)(F)(F)(F)F	dimethyl carbonate	0.45	-0.80	-0.44
methane	C	dimethyl carbonate	0.53	-0.30	-0.21
ethane	CC	dimethyl carbonate	-0.37	-1.88	-1.63
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	dimethyl carbonate	-3.88	-7.25	-7.01
ethene	C=C	dimethyl carbonate	-0.72	-2.19	-2.34
1,2-dichloroethane	ClCCCl	dimethyl carbonate	-4.07	-8.46	-7.62
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	dimethyl carbonate	-5.08	-7.59	-9.28
trichloroethene	ClC=C(Cl)Cl	dimethyl carbonate	-4.47	-8.17	-8.39
tetrachloroethene	ClC(Cl)=C(Cl)Cl	dimethyl carbonate	-5.11	-8.86	-9.47
ethanol	CCO	dimethyl carbonate	-3.10	-7.66	-7.10
butan-1-ol	CCCCO	dimethyl carbonate	-4.35	-9.51	-8.96
isobutanol	CC(C)CO	dimethyl carbonate	-4.38	-9.25	-9.06
methyl <i>tert</i> -butyl ether	COC(C)(C)C	dimethyl carbonate	-3.30	-6.75	-6.26
tetrahydrofuran	C1CCOC1	dimethyl carbonate	-3.71	-7.78	-6.83
tetrahydropyran	C1CCOCC1	dimethyl carbonate	-4.37	-8.86	-7.81
1,4-dioxane	C1COCCO1	dimethyl carbonate	-4.53	-9.09	-8.24
dimethyl carbonate	COC(=O)OC	dimethyl carbonate	-4.40	-9.01	-8.84
methyl ethyl ketone	CCC(C)=O	dimethyl carbonate	-4.02	-7.97	-7.84
2-hexanone	CCCCC(C)=O	dimethyl carbonate	-5.44	-9.77	-10.05
2-octanone	CCCCCCC(C)=O	dimethyl carbonate	-6.82	-11.47	-12.19

2-undecanone	CCCCCCCCC(C)=O	dimethyl carbonate		-8.70	-14.52	-15.00
cyclohexanone	O=C1CCCCC1	dimethyl carbonate		-5.83	-10.28	-10.50
2-methylcyclohexanone	CC1CCCCC1=O	dimethyl carbonate		-6.36	-10.58	-11.28
methyl acetate	COC(C)=O	dimethyl carbonate		-3.76	-7.72	-7.64
ethyl acetate	CCOC(C)=O	dimethyl carbonate		-4.35	-8.47	-8.54
hexyl acetate	CCCCCOC(C)=O	dimethyl carbonate		-6.88	-11.86	-12.34
vinyl acetate	CC(=O)OC=C	dimethyl carbonate		-4.80	-8.24	-9.56
1,2-dimethylbenzene	Cc1ccccc1C	dimethyl carbonate		-5.47	-9.69	-9.71
1,4-dimethylbenzene	Cc1ccc(C)cc1	dimethyl carbonate		-5.51	-9.44	-9.80
benzyl alcohol	OCc1ccccc1	dimethyl carbonate		-7.49	-13.32	-14.10
ethyl benzoate	CCOC(=O)c1ccccc1	dimethyl carbonate		-8.35	-14.17	-14.89
$\alpha$ -pinene	CC1=CCC2CC1C2(C)C	dimethyl carbonate		-6.37	-8.93	-10.63
$\beta$ -pinene	CC1(C)C2CCC(=C)C1C2	dimethyl carbonate		-6.36	-9.42	-10.61
anisole	COc1ccccc1	dimethyl carbonate		-6.13	-10.87	-11.03
phenetole	CCOc1ccccc1	dimethyl carbonate		-6.83	-11.61	-12.12
acetic acid	CC(O)=O	dimethyl carbonate		-4.66	-11.72	-10.39
1,2-epoxybutane	CCC1CO1	dimethyl carbonate		-3.81	-7.87	-7.06
helium	[He]	diethyl carbonate		2.32	3.28	2.68
neon	[Ne]	diethyl carbonate		2.21	2.59	2.37
argon	[Ar]	diethyl carbonate		1.18	0.49	0.66
xenon	[Xe]	diethyl carbonate		-0.23	-1.62	-1.29
sulfur hexafluoride	F[S](F)(F)(F)(F)F	diethyl carbonate		0.23	-0.57	-0.83
ethane	CC	diethyl carbonate		-0.44	-2.07	-2.00
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	diethyl carbonate		-3.96	-7.83	-7.39
ethene	C=C	diethyl carbonate		-0.78	-1.99	-2.70
1,2-dichloroethane	C1CCCl	diethyl carbonate		-4.12	-8.75	-7.97
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	diethyl carbonate		-4.89	-7.88	-9.10
1,2-dichloropropane	CC(Cl)CCl	diethyl carbonate		-5.00	-8.89	-9.44
1,3-dichloropropane	C1CCCl	diethyl carbonate		-4.93	-9.86	-9.31
1,4-dichlorobutane	C1CCCCl	diethyl carbonate		-5.92	-11.27	-10.91
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	diethyl carbonate		-6.17	-12.80	-11.06
<i>trans</i> -1,2-dichloroethene	C1C=C(Cl)Cl	diethyl carbonate		-3.83	-7.42	-7.63
trichloroethene	C1C=C(Cl)Cl	diethyl carbonate		-4.41	-8.48	-8.51
tetrachloroethene	ClC(Cl)=C(Cl)Cl	diethyl carbonate		-4.98	-9.24	-9.42
methanol	CO	diethyl carbonate		-2.43	-7.07	-6.27
ethanol	CCO	diethyl carbonate		-3.05	-7.88	-7.24
butan-1-ol	CCCCO	diethyl carbonate		-4.36	-9.99	-9.22
pentan-1-ol	CCCCCO	diethyl carbonate		-5.11	-11.09	-10.43
octan-1-ol	CCCCCCCCO	diethyl carbonate		-7.23	-14.21	-13.72
2-butanol	CCC(C)O	diethyl carbonate		-4.10	-9.23	-8.74
isobutanol	CC(C)CO	diethyl carbonate		-4.29	-9.57	-9.13
2-methyl-isopropanol	CC(C)(C)O	diethyl carbonate		-3.59	-8.60	-7.92
2-methyl-2-butanol	CCC(C)(C)O	diethyl carbonate		-4.15	-9.68	-8.75
3-methyl-1-butanol	CC(C)CCO	diethyl carbonate		-5.02	-10.54	-10.25
2-ethoxyethanol	CCOCCO	diethyl carbonate		-5.15	-10.15	-10.53
2-butoxyethanol	CCCCOCCO	diethyl carbonate		-6.40	-11.98	-12.44
methyl <i>tert</i> -butyl ether	COC(C)(C)C	diethyl carbonate		-3.22	-7.02	-6.35
tetrahydrofuran	C1CCOC1	diethyl carbonate		-3.77	-7.65	-7.19
tetrahydropyran	C1CCOCC1	diethyl carbonate		-4.43	-9.05	-8.18
1,4-dioxane	C1COCCO1	diethyl carbonate		-4.52	-9.00	-8.47
diethyl carbonate	CCOC(=O)OCC	diethyl carbonate		-4.96	-10.78	-9.62
acetone	CC(C)=O	diethyl carbonate		-3.28	-7.24	-6.94
methyl ethyl ketone	CCC(C)=O	diethyl carbonate		-4.07	-8.16	-8.19
2-pentanone	CCCC(C)=O	diethyl carbonate		-4.81	-9.03	-9.37
2-hexanone	CCCCC(C)=O	diethyl carbonate		-5.49	-10.10	-10.41
2-octanone	CCCCCCC(C)=O	diethyl carbonate		-6.91	-12.21	-12.62
2-undecanone	CCCCCCCCC(C)=O	diethyl carbonate		-8.84	-15.51	-15.53
cyclohexanone	O=C1CCCCC1	diethyl carbonate		-5.94	-10.54	-10.97
2-methylcyclohexanone	CC1CCCCC1=O	diethyl carbonate		-6.50	-10.78	-11.80
methyl acetate	COC(C)=O	diethyl carbonate		-3.62	-7.71	-7.58
ethyl acetate	CCOC(C)=O	diethyl carbonate		-4.28	-8.50	-8.62
butyl acetate	CCCCOC(C)=O	diethyl carbonate		-5.59	-10.40	-10.63
methyl propanoate	CCC(=O)OC	diethyl carbonate		-4.42	-8.54	-8.86
ethyl propanoate	CCOC(=O)CC	diethyl carbonate		-4.99	-9.39	-9.75
propyl propanoate	CCCOC(=O)CC	diethyl carbonate		-5.63	-10.33	-10.74
methyl butanoate	CCCC(=O)OC	diethyl carbonate		-5.13	-9.58	-10.00
ethyl butanoate	CCCC(=O)OCC	diethyl carbonate		-5.68	-10.01	-10.83
propyl butanoate	CCCOC(=O)CCC	diethyl carbonate		-6.33	-10.40	-11.86
benzene	c1ccccc1	diethyl carbonate		-4.04	-8.08	-7.65
toluene	Cc1ccccc1	diethyl carbonate		-4.73	-9.08	-8.73
ethylbenzene	CCc1ccccc1	diethyl carbonate		-5.50	-9.99	-9.95
1,2-dimethylbenzene	Cc1ccccc1C	diethyl carbonate		-5.35	-10.31	-9.68
1,4-dimethylbenzene	Cc1ccc(C)cc1	diethyl carbonate		-5.39	-10.06	-9.78
1,1,1,2-tetrafluoroethane	FCC(F)(F)F	diethyl carbonate		-0.73	-4.64	-1.84
2-phenylethanol	OCCc1ccccc1	diethyl carbonate		-7.90	-13.89	-14.78
ethyl benzoate	CCOC(=O)c1ccccc1	diethyl carbonate		-8.22	-14.57	-14.85
$\alpha$ -pinene	CC1=CCC2CC1C2(C)C	diethyl carbonate		-6.51	-9.71	-11.15
$\beta$ -pinene	CC1(C)C2CCC(=C)C1C2	diethyl carbonate		-6.51	-10.16	-11.16
p-cymene	CC(C)c1ccc(C)cc1	diethyl carbonate		-6.76	-11.74	-11.90
anisole	COc1ccccc1	diethyl carbonate		-5.99	-11.21	-10.97
4-fluorophenol	Oc1ccc(F)cc1	diethyl carbonate		-7.10	-15.85	-14.32
4-fluoroanisole	COc1ccc(F)cc1	diethyl carbonate		-6.22	-11.94	-11.73
xenon	[Xe]	acetic acid		-0.14	-1.37	-1.85

carbon monoxide	C=O	acetic acid	0.99	0.31	-0.33
pentane	CCCCC	acetic acid	-2.35	-5.20	-5.31
heptane	CCCCCCC	acetic acid	-3.79	-7.25	-7.61
octane	CCCCCCCC	acetic acid	-4.36	-8.19	-8.51
nonane	CCCCCCCCC	acetic acid	-5.21	-9.28	-9.90
decane	CCCCCCCCC	acetic acid	-5.96	-10.30	-11.09
undecane	CCCCCCCCCCC	acetic acid	-6.55	-11.30	-12.09
dodecane	CCCCCCCCCCCC	acetic acid	-7.26	-12.43	-13.23
tridecane	CCCCCCCCCCCCC	acetic acid	-7.87	-13.43	-14.30
2-methylpentane	CCCC(C)C	acetic acid	-2.93	-6.06	-6.25
3-methylpentane	CCC(C)CC	acetic acid	-2.92	-6.15	-6.25
2,2-dimethylbutane	CCC(C)(C)C	acetic acid	-2.35	-5.65	-5.24
2-methylhexane	CCCCC(C)C	acetic acid	-3.67	-7.01	-7.44
3-methylhexane	CCCC(C)CC	acetic acid	-3.61	-7.08	-7.34
2,4-dimethylpentane	CC(C)CC(C)C	acetic acid	-3.46	-6.59	-7.11
2,2,3-trimethylpentane	CCC(C)(C)(C)C	acetic acid	-3.57	-7.72	-7.27
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	acetic acid	-3.53	-7.11	-7.17
2,3,4-trimethylpentane	CC(C)(C)(C)C(C)C	acetic acid	-4.01	-7.69	-8.12
cyclohexane	C1CCCCC1	acetic acid	-3.50	-6.55	-6.74
cyclooctane	C1CCCCCCC1	acetic acid	-4.89	-8.65	-8.97
cyclodecane	C1CCCCCCCCC1	acetic acid	-6.24	-11.02	-11.34
methylcyclopentane	CC1CCCC1	acetic acid	-3.39	-6.27	-6.54
ethylcyclopentane	CCC1CCCC1	acetic acid	-4.09	-7.20	-7.64
methylcyclohexane	CC1CCCCC1	acetic acid	-4.11	-6.95	-7.74
ethylcyclohexane	CCC1CCCCC1	acetic acid	-4.82	-8.02	-8.88
1-ethylcyclopentene	CCC1=CCCC1	acetic acid	-4.39	-8.24	-8.19
methylidenecyclohexane	[CH2]=[C]1CC[CH2]CC1	acetic acid	-4.38	-7.52	-8.24
ethylidenecyclohexane	C[CH]=[C]1CC[CH2]CC1	acetic acid	-5.06	-8.83	-9.24
1-hexene	CCCCC=C	acetic acid	-3.32	-6.38	-6.81
1-heptene	CCCCC=C	acetic acid	-4.05	-7.43	-8.01
1,5-hexadiene	C=CCCC=C	acetic acid	-3.38	-6.47	-6.71
cyclohexene	C1CCC=CC1	acetic acid	-3.74	-7.01	-7.19
cycloheptene	C1CCC=CCC1	acetic acid	-4.45	-7.57	-8.31
1,3-cyclopentadiene	C1C=CC=C1	acetic acid	-3.32	-6.42	-6.74
1,4-cyclohexadiene	C1C=CCC=C1	acetic acid	-4.06	-7.42	-7.87
1,5-cyclooctadiene	C1CC=CCCC=C1	acetic acid	-5.36	-9.52	-9.78
cyclooctatetraene	C1=CC=CC=CC1	acetic acid	-5.44	-9.66	-9.89
ethanol	CCO	acetic acid	-3.90	-9.26	-9.24
1-propanol	CCCO	acetic acid	-4.65	-10.80	-10.48
butan-1-ol	CCCCO	acetic acid	-5.16	-11.70	-11.24
hexan-1-ol	CCCCCO	acetic acid	-6.48	-13.72	-13.40
heptan-1-ol	CCCCCCO	acetic acid	-7.24	-15.12	-14.68
octan-1-ol	CCCCCCCO	acetic acid	-8.11	-15.90	-16.05
nonan-1-ol	CCCCCCCCO	acetic acid	-8.74	-17.37	-16.99
decan-1-ol	CCCCCCCCCO	acetic acid	-9.26	-18.13	-17.82
ethylene glycol	OCCO	acetic acid	-6.14	-15.13	-14.78
ethyl acetate	CCOC(C)=O	acetic acid	-4.06	-8.60	-7.98
propyl acetate	CCCOC(C)=O	acetic acid	-4.84	-8.35	-9.32
butyl acetate	CCCCOC(C)=O	acetic acid	-5.44	-10.48	-10.33
ethyl propanoate	CCOC(=O)CC	acetic acid	-4.66	-9.32	-8.96
ethyl pentanoate	CCCCC(=O)OCC	acetic acid	-6.07	-11.02	-11.34
ethyl hexanoate	CCCCC(=O)OCC	acetic acid	-6.73	-12.00	-12.42
ethyl heptanoate	CCCCC(=O)OCC	acetic acid	-7.37	-12.87	-13.48
ethyl octanoate	CCCCC(=O)OCC	acetic acid	-7.93	-13.73	-14.51
ethyl decanoate	CCCCC(=O)OCC	acetic acid	-9.27	-16.04	-16.68
diisopropyl ether	CC(C)OC(C)C	acetic acid	-4.09	-8.14	-8.09
dibutyl ether	CCCCOCCCC	acetic acid	-5.78	-10.23	-10.73
tetrahydropyran	C1CCOCC1	acetic acid	-4.13	-9.07	-7.64
1,4-dioxane	C1COCCO1	acetic acid	-4.61	-9.52	-8.72
1-butanenitrile	CCCC#N	acetic acid	-4.81	-9.02	-8.18
dimethyl carbonate	COC(=O)OC	acetic acid	-3.93	-8.80	-7.73
diethyl carbonate	CCOC(=O)OCC	acetic acid	-4.76	-10.26	-9.10
benzene	c1ccccc1	acetic acid	-4.15	-7.65	-8.14
toluene	Cc1ccccc1	acetic acid	-4.86	-8.74	-9.25
m-xylene	Cc1cccc(C)c1	acetic acid	-5.54	-9.56	-10.32
p-xylene	Cc1ccc(C)cc1	acetic acid	-5.54	-9.61	-10.32
benzonitrile	N#Cc1ccccc1	acetic acid	-7.25	-11.64	-11.69
benzoic acid	OC(=O)c1ccccc1	acetic acid	-9.22	-17.57	-17.73
4-methylbenzoic acid	Cc1ccc(cc1)C(=O)=O	acetic acid	-9.93	-20.24	-18.87
2-hydroxybenzoic acid	OC(=O)c1ccccc1O	acetic acid	-10.55	-18.48	-21.28
acetic acid	CC(=O)=O	acetic acid	-5.33	-12.33	-11.79
propanoic acid	CCC(=O)=O	acetic acid	-5.81	-13.08	-12.61
butanoic acid	CCCC(=O)=O	acetic acid	-6.49	-13.59	-13.82
2-methylpropanoic acid	CC(C)C(=O)=O	acetic acid	-6.36	-12.96	-13.65
oxalic acid	OC(=O)C(=O)=O	acetic acid	-8.18	-16.77	-17.05
malonic acid	OC(=O)CC(=O)=O	acetic acid	-10.08	-23.03	-20.87
succinic acid	OC(=O)CCC(=O)=O	acetic acid	-10.41	-23.48	-21.87
glutaric acid	OC(=O)CCCC(=O)=O	acetic acid	-12.31	-25.03	-25.55
adipic acid	OC(=O)CCCCC(=O)=O	acetic acid	-12.54	-26.13	-26.01
pimelic acid	OC(=O)CCCCC(=O)=O	acetic acid	-13.66	-26.34	-27.71
suberic acid	OC(=O)CCCCC(=O)=O	acetic acid	-13.95	-28.25	-28.37
azelaic acid	OC(=O)CCCCC(=O)=O	acetic acid	-13.54	-30.19	-28.17
sebacic acid	OC(=O)CCCCC(=O)=O	acetic acid	-13.93	-30.16	-28.79

2-chloro-2-methylpropane	CC(C)(C)Cl	acetic acid	-3.33	-6.55	-6.87
2-bromo-2-methylpropane	CC(C)(C)Br	acetic acid	-3.56	-7.11	-7.28
N-methylpyrrole	Cn1cccc1	acetic acid	-5.20	-9.32	-10.06
pyrrole	[nH]1cccc1	acetic acid	-5.68	-10.55	-10.84
helium	[He]	chlorobenzene	1.98	2.40	1.95
neon	[Ne]	chlorobenzene	1.84	2.30	1.65
argon	[Ar]	chlorobenzene	0.73	0.11	0.05
xenon	[Xe]	chlorobenzene	-0.79	-2.08	-2.25
hydrogen	[H][H]	chlorobenzene	1.63	1.19	1.32
nitrogen	N#N	chlorobenzene	0.94	0.58	0.69
oxygen	O=O	chlorobenzene	0.66	0.15	-0.20
carbon monoxide	C=O	chlorobenzene	0.43	0.23	-0.46
methane	C	chlorobenzene	0.11	-0.61	-0.84
n-hexane	CCCCCC	chlorobenzene	-3.34	-6.94	-6.17
n-heptane	CCCCCCC	chlorobenzene	-4.12	-8.09	-7.42
n-nonane	CCCCCCCCC	chlorobenzene	-5.60	-10.33	-9.84
tetradecane	CCCCCCCCCCCCC	chlorobenzene	-8.98	-15.76	-15.38
dichloromethane	ClCCl	chlorobenzene	-3.59	-6.81	-6.58
tetrachloromethane	ClC(Cl)(Cl)Cl	chlorobenzene	-4.48	-7.80	-8.05
tetrachloroethene	ClC(Cl)=C(Cl)Cl	chlorobenzene	-4.73	-9.34	-8.49
trichloroethene	ClC=C(Cl)Cl	chlorobenzene	-4.63	-8.32	-8.28
diethyl ether	CCOCC	chlorobenzene	-3.93	-6.90	-7.22
dipropyl ether	CCCOCC	chlorobenzene	-5.15	-8.88	-9.20
methyl tert-butyl ether	COC(C)(C)C	chlorobenzene	-4.15	-7.67	-7.76
dimethoxymethane	COCOC	chlorobenzene	-4.31	-7.09	-7.79
1,2-dimethoxyethane	COCCOC	chlorobenzene	-5.12	-9.31	-9.00
tetrahydrofuran	C1CCOC1	chlorobenzene	-4.51	-8.30	-8.08
1,4-dioxane	C1COCCO1	chlorobenzene	-5.23	-9.35	-9.18
2-methyltetrahydrofuran	CC1CCCO1	chlorobenzene	-5.26	-8.02	-9.40
acetone	CC(C)=O	chlorobenzene	-4.17	-7.48	-7.62
butanone	CCC(C)=O	chlorobenzene	-4.80	-8.56	-8.56
pentan-2-one	CCCC(C)=O	chlorobenzene	-5.45	-9.47	-9.66
nonan-2-one	CCCCCCCC(C)=O	chlorobenzene	-8.20	-13.82	-14.08
acetophenone	CC(=O)c1ccccc1	chlorobenzene	-8.14	-13.17	-13.66
propyl acetate	CCCOC(C)=O	chlorobenzene	-5.40	-9.31	-9.55
butyl acetate	CCCCOC(C)=O	chlorobenzene	-6.02	-10.59	-10.60
methyl propionate	CCC(=O)OC	chlorobenzene	-4.79	-8.59	-8.47
propyl propionate	CCCOC(=O)CC	chlorobenzene	-5.89	-10.85	-10.36
ethyl benzoate	CCOC(=O)c1ccccc1	chlorobenzene	-8.81	-14.16	-14.76
propyl benzoate	CCCOC(=O)c1ccccc1	chlorobenzene	-9.48	-15.65	-15.93
butyl benzoate	CCCCOC(=O)c1ccccc1	chlorobenzene	-10.27	-16.50	-17.27
acetonitrile	CC#N	chlorobenzene	-4.65	-7.33	-7.52
propionitrile	CCC#N	chlorobenzene	-5.36	-8.60	-8.70
butyronitrile	CCCC#N	chlorobenzene	-5.88	-9.35	-9.51
triethylamine	CCN(CC)CC	chlorobenzene	-4.74	-8.52	-9.35
tri-n-butylamine	CCCCN(CCCC)CCCC	chlorobenzene	-7.92	-14.75	-15.21
dimethylformamide	CN(C)C=O	chlorobenzene	-6.24	-11.31	-11.68
N,N-dimethylacetamide	CN(C)C(C)=O	chlorobenzene	-6.94	-12.73	-13.09
methanol	CO	chlorobenzene	-3.04	-6.25	-6.49
ethanol	CCO	chlorobenzene	-3.65	-7.27	-7.58
propan-1-ol	CCCO	chlorobenzene	-4.36	-8.10	-8.76
butan-1-ol	CCCCO	chlorobenzene	-4.98	-8.56	-9.80
pentan-1-ol	CCCCCO	chlorobenzene	-5.79	-10.08	-11.17
hexan-1-ol	CCCCCCO	chlorobenzene	-6.40	-11.07	-12.17
octan-1-ol	CCCCCCCCO	chlorobenzene	-7.90	-13.50	-14.53
decan-1-ol	CCCCCCCCCO	chlorobenzene	-9.21	-15.88	-16.68
isopropanol	CC(C)O	chlorobenzene	-4.07	-7.61	-8.33
2-chlorophenol	Oc1ccccc1Cl	chlorobenzene	-7.91	-13.66	-13.72
2-methoxyphenol	COc1ccccc1O	chlorobenzene	-8.91	-13.56	-16.30
3-methoxyphenol	COc1cccc(O)c1	chlorobenzene	-9.61	-16.22	-17.34
4-methoxyphenol	COc1ccc(O)cc1	chlorobenzene	-9.74	-15.15	-17.58
benzene	c1ccccc1	chlorobenzene	-4.61	-8.08	-8.28
toluene	Cc1ccccc1	chlorobenzene	-5.35	-9.19	-9.46
ethylbenzene	CCc1ccccc1	chlorobenzene	-6.07	-10.28	-10.56
p-xylene	Cc1ccc(C)cc1	chlorobenzene	-6.06	-10.24	-10.60
anisole	COc1ccccc1	chlorobenzene	-6.50	-11.14	-11.07
biphenyl	c1ccc(cc1)c2ccccc2	chlorobenzene	-9.67	-15.51	-16.15
anthracene	c1ccc2cc3ccccc3cc2c1	chlorobenzene	-11.33	-18.59	-18.85
naphthalene	c1ccc2ccccc2c1	chlorobenzene	-8.17	-13.17	-13.98
1-chloronaphthalene	Clc1ccc2ccccc12	chlorobenzene	-9.26	-15.17	-15.50
chlorobenzene	Clc1ccccc1	chlorobenzene	-5.98	-9.80	-10.36
fluorobenzene	Fc1ccccc1	chlorobenzene	-4.98	-8.28	-8.90
bromobenzene	Brc1ccccc1	chlorobenzene	-6.30	-10.53	-10.83
iodobenzene	Ic1ccccc1	chlorobenzene	-7.33	-11.80	-12.04
1,3-dichlorobenzene	Clc1ccc(Cl)c1	chlorobenzene	-7.19	-11.16	-12.15
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	chlorobenzene	-7.21	-11.26	-12.19
1,2,4,5-tetrachlorobenzene	Clc1cc(Cl)c(Cl)cc1Cl	chlorobenzene	-9.02	-14.27	-15.08
hexachlorobenzene	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1	chlorobenzene	-10.00	-18.39	-16.94
1,3,5-trichlorobenzene	Clc1cc(Cl)cc(Cl)c1	chlorobenzene	-8.37	-12.20	-13.92
1,3,5-tribromobenzene	Brc1cc(Br)cc(Br)c1	chlorobenzene	-9.52	-15.26	-15.76
N-methylpyrrole	Cn1cccc1	chlorobenzene	-5.51	-9.75	-9.88
aniline	Nc1ccccc1	chlorobenzene	-7.36	-12.62	-12.51
pyridine	c1ccncc1	chlorobenzene	-5.89	-9.60	-9.75



3-methylpyridine	Cc1cccn1	chlorobenzene	-6.66	-10.75	-11.06
2-chloropyridine	Clc1cccn1	chlorobenzene	-7.20	-12.02	-11.83
3-chloropyridine	Clc1cccn1	chlorobenzene	-7.49	-11.22	-12.19
3-cyanopyridine	N#Cc1cccn1	chlorobenzene	-9.17	-12.88	-14.22
4-cyanopyridine	N#Cc1cccn1	chlorobenzene	-9.04	-12.55	-13.91
N-methylimidazole	Cn1ccn1	chlorobenzene	-7.40	-12.64	-12.54
indole	[nH]1ccc2ccccc12	chlorobenzene	-9.12	-15.29	-15.26
iodine	I	chlorobenzene	-5.86	-9.61	-9.65
pyrazole	[nH]1cccn1	chlorobenzene	-6.67	-11.33	-11.78
dimethyl sulfoxide	C[S](C)=O	chlorobenzene	-7.14	-12.21	-12.39
2,6-dimethoxyphenol	COc1cccc(OC)c1O	chlorobenzene	-9.21	-18.70	-16.42
N-methyl-2-pyrrolidone	CN1CCCC1=O	chlorobenzene	-8.21	-13.63	-14.83
cis-1,2-dichloroethene	Cl/C=C/Cl	chlorobenzene	-3.91	-7.23	-7.15
trans-1,2-dichloroethene	Cl/C=C/Cl	chlorobenzene	-4.23	-7.24	-7.54
ammonia	N	chlorobenzene	-2.20	-3.56	-4.33
hydrogen sulfide	S	chlorobenzene	-1.91	-2.89	-3.09
1,2-propylene oxide	CC1CO1	chlorobenzene	-3.90	-6.86	-7.13
water	O	chlorobenzene	-3.33	-4.76	-7.87
pentane	CCCCC	formamide	-1.16	-5.36	-4.24
hexane	CCCCCC	formamide	-1.65	-5.57	-4.97
heptane	CCCCCCC	formamide	-2.21	-6.48	-5.87
octane	CCCCCCCC	formamide	-2.61	-7.41	-6.52
nonane	CCCCCCCCC	formamide	-3.21	-9.20	-7.44
cyclohexane	C1CCCCC1	formamide	-2.73	-6.17	-6.66
methylcyclohexane	CC1CCCCC1	formamide	-3.01	-6.20	-7.07
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	formamide	-1.95	-7.30	-5.62
1-hexene	CCCC=C	formamide	-2.07	-6.20	-5.59
1-octene	CCCCCCC=C	formamide	-3.12	-7.70	-7.16
2,2,4-trimethyl-pent-3-ene	CC(C)(C)/C=C(C)/C	formamide	-2.49	-7.20	-6.23
1-chloropentane	CCCCCl	formamide	-3.53	-7.76	-7.98
1,5-dichloropentane	C1CCCCC1	formamide	-6.03	-10.88	-11.71
methanol	CO	formamide	-3.16	-8.74	-9.35
ethanol	CCO	formamide	-3.63	-9.58	-10.16
butan-1-ol	CCCCO	formamide	-4.52	-11.59	-11.54
pentan-1-ol	CCCCCO	formamide	-5.19	-12.53	-12.68
hexan-1-ol	CCCCCO	formamide	-5.48	-13.16	-13.05
heptan-1-ol	CCCCCO	formamide	-6.08	-14.38	-14.04
decan-1-ol	CCCCCCCCCO	formamide	-7.60	-17.03	-16.37
1,2-butanediol	CCC(O)CO	formamide	-6.87	-16.90	-17.39
1,3-butanediol	CC(O)CCO	formamide	-6.91	-17.07	-17.24
1,5-pentanediol	OCCCCO	formamide	-8.91	-20.02	-20.36
cyclohexanol	OC1CCCCC1	formamide	-6.08	-13.67	-13.78
cis-1,2-cyclohexanediol	O[C@H]1CCCC[C@H]1O	formamide	-7.48	-16.80	-18.36
2,2,2-trifluoroethanol	OCC(F)(F)F	formamide	-3.87	-10.82	-11.29
1,4-dioxane	C1COCCO1	formamide	-4.59	-9.71	-9.83
12-crown-4	C1COCCOCCOCCO1	formamide	-8.58	-19.40	-18.22
15-crown-5	C1COCCOCCOCCOCCO1	formamide	-10.31	-24.47	-21.76
benzo-15-crown-5	C1COCCOCCOCCOCCO1	formamide	-13.65	-29.22	-27.79
acetonitrile	CC#N	formamide	-3.58	-7.80	-7.01
benzene	c1ccccc1	formamide	-3.15	-7.03	-7.21
ethylbenzene	CCc1ccccc1	formamide	-4.25	-8.80	-8.81
propylbenzene	CCCc1ccccc1	formamide	-4.77	-9.20	-9.57
isopropylbenzene	CC(C)c1ccccc1	formamide	-4.68	-8.80	-9.45
o-xylene	Cc1ccccc1C	formamide	-4.17	-8.80	-8.76
m-xylene	Cc1ccc(C)cc1	formamide	-4.22	-8.39	-8.81
p-xylene	Cc1ccc(C)cc1	formamide	-4.23	-8.39	-8.82
chlorobenzene	Clc1ccccc1	formamide	-4.66	-8.77	-9.60
bromobenzene	Brc1ccccc1	formamide	-4.98	-9.63	-10.04
aniline	Nc1ccccc1	formamide	-6.48	-12.64	-13.19
naphthalene	c1ccc2ccccc2c1	formamide	-6.24	-11.83	-12.00
formamide	NC=O	formamide	-6.72	-14.39	-14.03
methylformamide	CNC=O	formamide	-6.15	-13.44	-13.16
N-methylacetamide	CNC(C)=O	formamide	-6.75	-14.85	-14.77
N-methylpropanamide	CCC(=O)NC	formamide	-7.41	-15.69	-16.04
dimethylformamide	CN(C)C=O	formamide	-5.57	-12.70	-12.11
N,N-diethylformamide	CCN(CC)C=O	formamide	-6.51	-13.57	-14.17
N,N-dimethylacetamide	CN(C)C(C)=O	formamide	-6.24	-14.07	-13.60
N,N-diethylacetamide	CCN(CC)C(C)=O	formamide	-6.97	-15.04	-15.39
N-methylpyrrole	Cn1cccn1	formamide	-4.41	-8.89	-9.86
pyrrole	[nH]1cccn1	formamide	-4.69	-10.71	-9.99
N-methylimidazole	Cn1ccn1	formamide	-6.80	-13.87	-13.26
water	O	formamide	-4.68	-10.23	-12.97
acetic acid	CC(O)=O	formamide	-6.24	-13.23	-14.24
formic acid	OC=O	formamide	-5.58	-12.97	-13.21
pyridine	c1ccncc1	formamide	-5.10	-9.61	-9.90
2-methylpyridine	Cc1cccn1	formamide	-5.71	-10.16	-11.11
1,2-dihydroxybenzene	Oc1ccccc1O	formamide	-8.26	-19.24	-17.52
1,3-dihydroxybenzene	Oc1ccc(O)c1	formamide	-10.15	-19.72	-21.41
1,4-dihydroxybenzene	Oc1ccc(O)cc1	formamide	-10.34	-21.85	-21.70
1,2-diaminobenzene	Nc1ccccc1N	formamide	-8.29	-18.36	-18.11
1,4-diaminobenzene	Nc1ccc(N)cc1	formamide	-10.06	-20.51	-20.45
pentane	CCCCC	methylformamide	-2.05	-4.53	-4.53
hexane	CCCCCC	methylformamide	-2.43	-6.29	-5.07

heptane	CCCCCCC	methylformamide	-2.79	-7.39	-5.57
octane	CCCCCCCC	methylformamide	-3.13	-8.39	-6.15
nonane	CCCCCCCCC	methylformamide	-3.52	-9.42	-6.68
decane	CCCCCCCCC	methylformamide	-3.92	-10.42	-7.28
cyclohexane	C1CCCCC1	methylformamide	-3.53	-6.81	-6.78
methylcyclopentane	CC1CCCC1	methylformamide	-3.45	-6.47	-6.65
methylcyclohexane	CC1CCCCC1	methylformamide	-3.68	-7.40	-6.87
1-pentene	CCCC=C	methylformamide	-2.46	-5.42	-5.16
1-hexene	CCCCC=C	methylformamide	-2.74	-6.46	-5.50
1-octene	CCCCCCC=C	methylformamide	-3.26	8.61	-6.10
cyclohexene	C1CCC=CC1	methylformamide	-3.84	-7.25	-7.36
dichloromethane	C1CC1	methylformamide	-3.65	-7.96	-7.50
chloroform	ClC(Cl)Cl	methylformamide	-4.08	-8.79	-7.96
2-chloro-2-methylpropane	CC(C)(C)Cl	methylformamide	-3.63	-6.57	-7.44
benzene	c1ccccc1	methylformamide	-3.93	-7.82	-7.51
toluene	Cc1ccccc1	methylformamide	-4.53	-8.70	-8.47
ethylbenzene	CCc1ccccc1	methylformamide	-4.94	-9.66	-9.04
1,2-dimethylbenzene	Cc1ccccc1C	methylformamide	-4.99	-9.70	-9.19
1,3-dimethylbenzene	Cc1cccc(C)c1	methylformamide	-5.06	-9.63	-9.33
1,4-dimethylbenzene	Cc1ccc(C)cc1	methylformamide	-5.07	-9.58	-9.33
fluorobenzene	Fc1ccccc1	methylformamide	-4.51	-8.29	-8.65
naphthalene	c1ccc2ccccc2c1	methylformamide	-6.86	-12.83	-12.22
ethanol	CCO	methylformamide	-4.44	-9.26	-10.21
isopropanol	CC(C)O	methylformamide	-4.57	-9.82	-10.34
1,2-ethanediol	OCCO	methylformamide	-6.36	-15.68	-14.62
1,3-butanediol	CC(O)CCO	methylformamide	-7.15	-16.75	-15.89
butanone	CCC(C)=O	methylformamide	-4.34	-8.13	-8.43
2-pentanone	CCCC(C)=O	methylformamide	-4.72	-9.02	-9.02
acetonitrile	CC#N	methylformamide	-4.25	-7.52	-7.62
propionitrile	CCC#N	methylformamide	-4.83	-8.18	-8.59
diethyl ether	CCOCC	methylformamide	-3.18	-6.16	-6.57
diisopropyl ether	CC(C)OC(C)C	methylformamide	-3.73	-7.30	-7.30
methyl tert-butyl ether	COC(C)(C)C	methylformamide	-3.47	-6.98	-7.01
ethyl tert-butyl ether	CCOC(C)(C)C	methylformamide	-3.76	-7.57	-7.44
methyl tert-amyl ether	CCC(C)(C)OC	methylformamide	-3.60	-8.24	-7.13
tetrahydrofuran	C1CCOC1	methylformamide	-4.16	-7.71	-8.03
1,4-dioxane	C1COCCO1	methylformamide	-5.45	-9.02	-10.15
ethyl acetate	CCOC(C)=O	methylformamide	-5.10	-8.27	-9.41
pyridine	c1ccncc1	methylformamide	-5.62	-9.84	-10.07
3-methylpyridine	Cc1ccncc1	methylformamide	-6.32	-11.08	-11.31
methylformamide	CNC=O	methylformamide	-6.69	-13.00	-13.45
4-fluorophenol	Oc1ccc(F)cc1	methylformamide	-8.27	-17.66	-16.77
4-nitrophenol	Oc1ccc(cc1)[N+](=O)=O	methylformamide	-11.68	-22.83	-22.16
4-fluoroanisole	COc1ccc(F)cc1	methylformamide	-6.44	-11.53	-12.08
phenol	Oc1ccccc1	methylformamide	-7.40	-15.87	-14.82
1-naphthol	Oc1cccc2ccccc12	methylformamide	-10.01	-20.39	-18.88
dimethylformamide	CN(C)C=O	methylformamide	-6.11	-11.31	-11.90
N,N-dimethylacetamide	CN(C)C(C)=O	methylformamide	-6.63	-12.51	-12.97
15-crown-5	C1COCOCOCOCOCOC1	methylformamide	-10.09	-20.63	-19.79
benzo-15-crown-5	C1COCOCOc2ccccc2OCCOCOC1	methylformamide	-13.17	-24.18	-25.22
pentane	CCCCC	triethylamine	-3.37	-6.30	-6.76
hexane	CCCCCC	triethylamine	-4.07	-7.46	-7.86
heptane	CCCCCCC	triethylamine	-4.77	-8.64	-8.93
octane	CCCCCCCC	triethylamine	-5.40	-9.81	-9.89
nonane	CCCCCCCCC	triethylamine	-6.14	-10.95	-11.07
decane	CCCCCCCCC	triethylamine	-6.84	-12.10	-12.16
dodecane	CCCCCCCCCCC	triethylamine	-8.15	-14.47	-14.15
3-ethylpentane	CCC(CC)CC	triethylamine	-4.67	-8.35	-8.80
cyclohexane	C1CCCCC1	triethylamine	-4.13	-7.74	-7.49
1-hexyne	CCCCC#C	triethylamine	-4.11	-8.26	-7.73
1-octyne	CCCCCCC#C	triethylamine	-5.46	-10.54	-9.77
2-octyne	CCCCCCC#CC	triethylamine	-5.41	-10.73	-9.68
4-octyne	CCCC#CCCC	triethylamine	-5.38	-10.29	-9.63
acetone	CC(C)=O	triethylamine	-2.94	-6.02	-5.96
2-heptanone	CCCCC(C)=O	triethylamine	-5.67	-10.52	-10.14
4-heptanone	CCCC(=O)CCC	triethylamine	-5.71	-10.49	-10.24
2-nonanone	CCCCCCC(C)=O	triethylamine	-7.02	-12.65	-12.23
5-nonanone	CCCCC(=O)CCCC	triethylamine	-6.92	-12.59	-12.05
cyclohexanone	O=C1CCCCC1	triethylamine	-5.79	-9.89	-10.54
dibutyl ether	CCCCOCCCC	triethylamine	-6.10	-10.74	-10.87
butyl methyl ether	CCCCOC	triethylamine	-4.26	-7.72	-8.08
methyl tert butyl ether	COC(C)(C)C	triethylamine	-3.59	-7.35	-6.92
methyl heptyl ether	CCCCCCCOC	triethylamine	-6.29	-11.14	-11.18
1-fluorooctane	CCCCCCCCF	triethylamine	-6.06	-11.74	-10.95
chloroform	ClC(Cl)Cl	triethylamine	-4.36	-10.46	-8.36
1-chlorooctane	CCCCCCCCCl	triethylamine	-6.80	-12.52	-11.98
m-cresol	Cc1ccc(O)cc1	triethylamine	-7.08	-19.58	-13.36
methanol	CO	triethylamine	-2.86	-10.09	-6.90
ethanol	CCO	triethylamine	-3.59	-10.96	-8.10
1-propanol	CCCO	triethylamine	-4.27	-12.28	-9.15
1-butanol	CCCCO	triethylamine	-4.85	-13.34	-10.02
1-hexanol	CCCCCO	triethylamine	-6.27	-15.87	-12.21
1-octanol	CCCCCCCCO	triethylamine	-7.45	-18.18	-13.92

benzene	c1ccccc1	triethylamine	-4.39	-7.82	-8.23
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	triethylamine	-6.11	-11.18	-10.80
(trifluoromethyl)benzene	FC(F)(F)c1ccccc1	triethylamine	-5.18	-8.95	-9.64
nitrobenzene	[O-][N+](=O)c1ccccc1	triethylamine	-6.24	-12.15	-11.39
formamide	NC=O	triethylamine	-5.15	-15.13	-10.89
methylformamide	CNC=O	triethylamine	-5.43	-12.33	-11.00
4-fluoroanisole	COc1ccc(F)cc1	triethylamine	-5.92	-11.36	-10.82
triethylamine	CCN(CC)CC	triethylamine	-4.44	-8.32	-8.28
aniline	Nc1ccccc1	triethylamine	-6.82	-13.78	-12.58
pyridine	c1ccncc1	triethylamine	-4.87	-8.59	-8.41
pentane	CCCCC	benzotrifluoride	-2.94	-5.65	-5.56
hexane	CCCCCC	benzotrifluoride	-3.54	-6.74	-6.42
heptane	CCCCCCC	benzotrifluoride	-4.16	-7.83	-7.33
nonane	CCCCCCCCC	benzotrifluoride	-5.39	-9.99	-9.15
hexadecane	CCCCCCCCCCCCCCC	benzotrifluoride	-9.68	-17.44	-15.55
2,2-dimethylbutane	CCC(C)(C)C	benzotrifluoride	-3.07	-5.59	-5.84
3-ethylpentane	CCC(CC)CC	benzotrifluoride	-4.05	-7.59	-7.24
cyclohexane	C1CCCCC1	benzotrifluoride	-4.10	-6.93	-7.10
1-hexene	CCCCC=C	benzotrifluoride	-3.75	-6.85	-6.71
1-octene	CCCCCCC=C	benzotrifluoride	-4.97	-9.05	-8.50
diethyl ether	CCOCC	benzotrifluoride	-4.10	-6.78	-7.50
methyl butyl ether	CCCCOC	benzotrifluoride	-4.68	-7.93	-8.35
dibutyl ether	CCCCOCCCC	benzotrifluoride	-6.14	-10.53	-10.43
methyl ethyl ketone	CCC(C)=O	benzotrifluoride	-4.81	-8.56	-8.82
2-heptanone	CCCCCC(C)=O	benzotrifluoride	-6.50	-11.68	-11.29
4-heptanone	CCCC(=O)CCC	benzotrifluoride	-6.28	-11.33	-10.84
2-nonanone	CCCCCCCC(C)=O	benzotrifluoride	-7.56	-13.82	-12.79
5-nonanone	CCCCC(=O)CCCC	benzotrifluoride	-7.50	-13.32	-12.70
cyclohexanone	O=C1CCCCC1	benzotrifluoride	-6.42	-11.17	-11.11
1-butanol	CCCCO	benzotrifluoride	-4.94	-8.14	-9.78
1-octanol	CCCCCCCCO	benzotrifluoride	-7.51	-12.46	-13.63
3-methyl-2-butanol	CC(C)C(C)O	benzotrifluoride	-5.17	-8.08	-10.23
benzene	c1ccccc1	benzotrifluoride	-4.54	-7.84	-7.93
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	benzotrifluoride	-6.17	-11.32	-10.40
pyridine	c1ccncc1	benzotrifluoride	-5.95	-9.35	-9.65
aniline	Nc1ccccc1	benzotrifluoride	-7.38	-11.36	-12.91
nitrobenzene	[O-][N+](=O)c1ccccc1	benzotrifluoride	-7.31	-12.79	-12.74
benzotrifluoride	FC(F)(F)c1ccccc1	benzotrifluoride	-5.41	-9.03	-9.10
3-methylphenol	Cc1ccc(O)c1	benzotrifluoride	-7.63	-11.21	-13.79
triethylamine	CCN(CC)CC	benzotrifluoride	-4.52	-8.59	-8.16
helium	[He]	ethylene glycol	2.02	1.43	1.92
xenon	[Xe]	ethylene glycol	0.48	-1.74	-1.62
hexane	CCCCCC	ethylene glycol	-2.07	-5.47	-5.79
heptane	CCCCCCC	ethylene glycol	-2.63	-6.48	-6.68
octane	CCCCCCCC	ethylene glycol	-3.12	-7.39	-7.48
nonane	CCCCCCCCC	ethylene glycol	-3.99	-8.29	-8.93
cyclohexane	C1CCCCC1	ethylene glycol	-2.86	-6.17	-7.01
acetylene	C#C	ethylene glycol	-0.67	-4.21	-3.82
2-chloro-2-methylpropane	CC(C)(C)Cl	ethylene glycol	-2.71	-5.57	-6.69
2-chloro-2-methylbutane	CCC(C)(C)Cl	ethylene glycol	-3.44	-6.88	-7.87
3-chloro-3-methylpentane	CCC(C)(C)CC	ethylene glycol	-4.09	-8.08	-8.95
diethyl ether	CCOCC	ethylene glycol	-2.77	-6.12	-6.83
tetrahydrofuran	C1CCOC1	ethylene glycol	-3.37	-7.48	-7.77
propanone	CC(C)=O	ethylene glycol	-3.01	-6.88	-7.16
butanone	CCC(C)=O	ethylene glycol	-3.58	-7.48	-7.97
2-hexanone	CCCCC(C)=O	ethylene glycol	-4.59	-9.87	-9.54
methyl acetate	COC(C)=O	ethylene glycol	-3.36	-6.96	-7.52
ethyl acetate	CCOC(C)=O	ethylene glycol	-3.67	-7.46	-8.08
propyl acetate	CCCOC(C)=O	ethylene glycol	-4.11	-8.37	-8.88
acetonitrile	CC#N	ethylene glycol	-3.70	-7.00	-7.16
propionitrile	CCC#N	ethylene glycol	-4.49	-7.79	-8.58
butyronitrile	CCCC#N	ethylene glycol	-5.11	-8.25	-9.69
triethylamine	CCN(CC)CC	ethylene glycol	-3.72	-11.35	-9.83
nitromethane	C[N+](=O)=O	ethylene glycol	-4.04	-8.22	-9.06
methanol	CO	ethylene glycol	-3.43	-8.94	-9.76
ethanol	CCO	ethylene glycol	-3.91	-9.82	-10.59
1-propanol	CCCO	ethylene glycol	-4.48	-10.78	-11.52
1-butanol	CCCCO	ethylene glycol	-4.94	-11.69	-12.26
2-butanol	CCC(C)O	ethylene glycol	-4.49	-11.14	-11.39
1-pentanol	CCCCCO	ethylene glycol	-5.31	-12.55	-12.79
1-hexanol	CCCCCCO	ethylene glycol	-6.42	-13.38	-14.68
1-heptanol	CCCCCCCO	ethylene glycol	-6.91	-14.34	-15.54
ethylene glycol	OCCO	ethylene glycol	-6.36	-15.77	-16.73
toluene	Cc1ccccc1	ethylene glycol	-4.00	-8.44	-8.59
p-xylene	Cc1ccc(C)cc1	ethylene glycol	-4.54	-9.25	-9.43
m-xylene	Cc1ccc(C)c1	ethylene glycol	-4.54	-9.32	-9.43
naphthalene	c1ccc2ccccc2c1	ethylene glycol	-6.70	-12.86	-12.88
biphenyl	c1ccc(cc1)c2ccccc2	ethylene glycol	-8.14	-15.61	-14.77
fluorobenzene	Fc1ccccc1	ethylene glycol	-3.94	-7.98	-8.64
chlorobenzene	Clc1ccccc1	ethylene glycol	-4.91	-9.27	-10.05
bromobenzene	Brc1ccccc1	ethylene glycol	-5.29	-10.49	-10.65
acetophenone	CC(=O)c1ccccc1	ethylene glycol	-6.75	-11.62	-12.56
N-methylimidazole	Cn1ccnc1	ethylene glycol	-7.14	-14.29	-13.77

<i>n</i> -methylpyrrole	Cn1cccc1	ethylene glycol		-4.71	-8.80	-10.43
pyridine	c1ccccc1	ethylene glycol		-5.37	-10.97	-10.46
piperidine	C1CCNCC1	ethylene glycol		-5.41	-12.55	-12.46
dimethyl sulfoxide	C[S](C)=O	ethylene glycol		-7.07	-13.43	-13.41
2-phenylethanol	OCCc1ccccc1	ethylene glycol		-8.34	-15.68	-17.00
butylamine	CCCCN	ethylene glycol		-4.83	-12.72	-12.27
hexylamine	CCCCCN	ethylene glycol		-5.88	-14.24	-14.35
dipropylamine	CCCNCCC	ethylene glycol		-4.83	-13.50	-12.52
dibutylamine	CCCCNCCCC	ethylene glycol		-5.71	-14.94	-14.24
triethylamine	CCN(CC)CC	ethylene glycol		-3.72	-11.35	-9.83
<i>n</i> -octane	CCCCCCCC	pyridine		-4.71	-7.98	-8.46
<i>n</i> -tetradecane	CCCCCCCCCCCCCCC	pyridine		-8.63	-13.98	-14.78
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	pyridine		-3.85	-6.60	-7.12
dichloromethane	CICCl	pyridine		-3.72	-7.29	-6.78
trichloromethane	ClC(Cl)Cl	pyridine		-4.69	-9.18	-8.49
tetrachloromethane	ClC(Cl)(Cl)Cl	pyridine		-4.79	-7.86	-8.75
<i>cis</i> -1,2-dichloroethene	Cl/C=C/Cl	pyridine		-4.06	-8.03	-7.37
<i>trans</i> -1,2-dichloroethene	Cl/C=C\Cl	pyridine		-4.41	-7.53	-7.84
trichloroethylene	ClC=C(Cl)Cl	pyridine		-4.97	-8.46	-8.99
1-chlorobutane	CCCCCl	pyridine		-4.31	-7.60	-7.73
acetone	CC(C)=O	pyridine		-4.08	-7.34	-7.41
butanone	CCC(C)=O	pyridine		-4.65	-8.29	-8.21
2-pentanone	CCCC(C)=O	pyridine		-5.20	-9.13	-9.11
2-hexanone	CCCCC(C)=O	pyridine		-5.81	-10.33	-10.01
2-octanone	CCCCCCC(C)=O	pyridine		-7.18	-12.26	-12.16
diethyl ether	CCOCC	pyridine		-3.59	-6.64	-6.34
2,5-dioxahexane	COCCOC	pyridine		-5.14	-8.99	-8.87
2,5,8-trioxanonane	COCCOCCOC	pyridine		-7.71	-12.14	-13.64
2,5,8,11-tetraoxadodecane	COCCOCCOCCOC	pyridine		-9.59	-16.11	-16.61
2,5,8,11,14-pentaoxapentadecane	COCCOCCOCCOCCOC	pyridine		-11.32	-19.60	-19.65
1,4-dioxane	C1COCCO1	pyridine		-5.07	-9.42	-8.58
12-crown-4	C1COCCOCCOCCO1	pyridine		-8.92	-16.20	-16.36
15-crown-5	C1COCCOCCOCCOCCO1	pyridine		-10.69	-18.86	-19.94
18-crown-6	C1COCCOCCOCCOCCOCCO1	pyridine		-12.37	-24.28	-23.22
methanol	CO	pyridine		-3.95	-9.54	-8.57
ethanol	CCO	pyridine		-4.44	-9.97	-9.37
propan-1-ol	CCCO	pyridine		-5.01	-10.90	-10.25
butan-1-ol	CCCCO	pyridine		-5.57	-11.26	-11.16
hexan-1-ol	CCCCCO	pyridine		-6.88	-14.22	-13.30
octan-1-ol	CCCCCOO	pyridine		-8.32	-15.97	-15.53
2-methylbutan-2-ol	CCC(C)(C)O	pyridine		-5.10	-10.61	-10.35
ethane-1,2-diol	OCCO	pyridine		-6.94	-16.87	-14.84
benzene	c1ccccc1	pyridine		-4.51	-8.37	-7.88
toluene	Cc1ccccc1	pyridine		-5.21	-9.08	-9.04
fluorobenzene	Fc1ccccc1	pyridine		-4.94	-8.25	-8.69
chlorobenzene	Clc1ccccc1	pyridine		-5.92	-9.58	-10.14
bromobenzene	Brc1ccccc1	pyridine		-6.14	-10.37	-10.40
iodobenzene	Ic1ccccc1	pyridine		-7.09	-11.38	-11.56
1,2-dichlorobenzene	Clc1ccccc1Cl	pyridine		-7.05	-11.74	-11.99
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	pyridine		-7.24	-11.16	-12.21
1,2,4,5-tetrachlorobenzene	Clc1cc(Cl)c(Cl)cc1Cl	pyridine		-9.22	-14.20	-15.46
2-methoxyphenol	COc1ccccc1O	pyridine		-9.37	-17.42	-17.37
3-methoxyphenol	COc1cccc(O)c1	pyridine		-10.35	-21.65	-19.17
4-methoxyphenol	COc1ccc(O)cc1	pyridine		-10.51	-20.75	-19.46
2-nitrophenol	Oc1ccccc1[N+](=O)[O-]	pyridine		-9.47	-15.08	-17.13
4-nitrophenol	Oc1ccc(cc1)[N+](=O)[O-]	pyridine		-11.81	-23.40	-21.79
3-chlorophenol	Oc1cccc(Cl)c1	pyridine		-9.95	-19.67	-18.42
4-chlorophenol	Oc1ccc(Cl)cc1	pyridine		-9.94	-19.96	-18.39
4-fluorophenol	Oc1ccc(F)cc1	pyridine		-9.10	-18.67	-17.53
3-bromophenol	Oc1cccc(Br)c1	pyridine		-10.37	-19.57	-19.17
methyl-2-hydroxybenzoate	COC(=O)c1ccccc1O	pyridine		-9.72	-13.03	-17.61
methyl-4-hydroxybenzoate	COC(=O)c1ccc(O)cc1	pyridine		-11.98	-22.01	-21.77
ethyl-4-hydroxybenzoate	CCOC(=O)c1ccc(O)cc1	pyridine		-12.48	-22.11	-22.49
propyl-4-hydroxybenzoate	CCOC(=O)c1ccc(O)cc1	pyridine		-13.12	-26.82	-23.53
4-hydroxybenzaldehyde	Oc1ccc(C=O)cc1	pyridine		-11.25	-22.78	-20.54
1,3-dihydroxybenzene	Oc1ccc(O)c1	pyridine		-11.64	-25.48	-22.60
hexachlorobenzene	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	pyridine		-10.20	-17.64	-17.43
aniline	Nc1ccccc1	pyridine		-8.34	-15.11	-14.81
<i>n</i> -methylaniline	CNc1ccccc1	pyridine		-7.92	-14.34	-14.04
<i>n</i> -ethylaniline	CCNc1ccccc1	pyridine		-8.46	-15.18	-15.12
<i>N,N</i> -dimethylaniline	CN(C)c1ccccc1	pyridine		-7.68	-12.81	-13.50
nitrobenzene	[O-][N+](=O)c1ccccc1	pyridine		-7.94	-12.98	-13.60
4-chloronitrobenzene	[O-][N+](=O)c1ccc(Cl)cc1	pyridine		-9.12	-14.36	-15.44
phenol	Oc1ccccc1	pyridine		-8.44	-17.83	-15.89
2,4-di- <i>tert</i> -butylphenol	CC(C)(C)c1ccc(O)c(c1)C(C)(C)C	pyridine		-11.46	-22.73	-20.81
2,6-di- <i>tert</i> -butylphenol	CC(C)(C)c1ccc(cc1O)C(C)(C)C	pyridine		-10.87	-19.31	-20.17
4-fluoroanisole	COc1ccc(F)cc1	pyridine		-7.33	-11.57	-13.00
2-hydroxyacetophenone	OCC(=O)c1ccccc1	pyridine		-10.57	-13.77	-18.94
4-hydroxyacetophenone	CC(=O)c1ccc(O)cc1	pyridine		-11.94	-23.97	-21.67
benzophenone	O=C(c1ccccc1)c2ccccc2	pyridine		-11.81	-18.12	-19.01
<i>cis</i> -azobenzene	c1ccc(cc1)N=Nc2ccccc2	pyridine		-11.49	-16.99	-18.01
biphenyl	c1ccc(cc1)c2ccccc2	pyridine		-9.54	-15.77	-15.73

naphthalene	c1ccc2ccccc2c1	pyridine	-7.99	-13.15	-13.49
1-chloronaphthalene	Clc1ccc2ccccc12	pyridine	-9.07	-14.46	-15.05
1-nitronaphthalene	[O-][N+](=O)c1ccc2ccccc12	pyridine	-10.78	-18.24	-17.77
1-naphthol	Oc1ccc2ccccc12	pyridine	-11.88	-22.90	-21.43
anthracene	c1ccc2cc3ccccc3cc2c1	pyridine	-11.28	-18.76	-18.68
benzaldehyde	O=Cc1ccccc1	pyridine	-7.19	-12.21	-12.00
4-methoxybenzaldehyde	COc1ccc(C=O)cc1	pyridine	-9.37	-14.22	-15.79
2-chlorobenzaldehyde	Clc1ccccc1C=O	pyridine	-8.69	-13.31	-14.47
9-anthraldehyde	O=Cc1c2ccccc2cc3ccccc13	pyridine	-13.74	-19.96	-22.40
piperidine	C1CCNCC1	pyridine	-6.02	-9.03	-11.16
pyrrole	[nH]1cccc1	pyridine	-6.47	-12.95	-11.59
<i>n</i> -methylpyrrole	Cn1cccc1	pyridine	-5.52	-9.80	-9.74
pyridine	c1ccncc1	pyridine	-6.12	-9.61	-10.01
imidazole	[nH]1ccnc1	pyridine	-9.36	-16.85	-16.68
1,3-diazine	c1ccncc1	pyridine	-8.08	-11.81	-13.21
1,4-diazine	c1ccncc1	pyridine	-7.18	-9.56	-11.12
indole	[nH]1ccc2ccccc12	pyridine	-9.94	-18.98	-17.19
<i>n</i> -methylindole	Cn1ccc2ccccc12	pyridine	-9.15	-14.99	-15.55
2-pyrrolidone	O=C1CCCN1	pyridine	-9.26	-17.66	-16.91
<i>N</i> -methyl-2-pyrrolidone	CN1CCCN1=O	pyridine	-8.00	-13.50	-14.10
methylformamide	CNC=O	pyridine	-7.37	-13.48	-14.05
dimethylformamide	CN(C)C=O	pyridine	-6.20	-11.33	-11.33
acetamide	CC(N)=O	pyridine	-8.06	-15.58	-15.58
<i>n</i> -methylacetamide	CNC(C)=O	pyridine	-7.94	-16.71	-15.04
<i>N,N</i> -dimethylacetamide	CN(C)C(C)=O	pyridine	-6.87	-12.36	-12.67
carbazole	[nH]1c2ccccc2c3ccccc13	pyridine	-13.29	-22.73	-22.50
water	O	pyridine	-4.15	-10.99	-9.70
$\gamma$ -butyrolactam	O=C1CCCN1	pyridine	-9.26	-17.69	-16.91
<i>N</i> -methylbutyrolactam	CN1CCCC1=O	pyridine	-8.00	-14.01	-14.10
<i>N</i> -methylvalerolactam	CN1CCCCC1=O	pyridine	-8.46	-15.01	-14.85
$\epsilon$ -caprolactam	O=C1CCCCCN1	pyridine	-9.79	-17.69	-17.56
hydrogen	[H][H]	methyl acetate	1.05	1.21	0.46
nitrogen	N#N	methyl acetate	1.03	0.68	0.80
oxygen	O=O	methyl acetate	0.08	0.34	-1.71
carbon monoxide	C=O	methyl acetate	0.42	0.34	-0.41
methane	C	methyl acetate	0.41	-0.33	-0.25
ethane	CC	methyl acetate	-0.55	-2.06	-1.77
pentane	CCCCC	methyl acetate	-2.73	-5.20	-5.14
hexane	CCCCCC	methyl acetate	-3.39	-5.78	-6.15
heptane	CCCCCCC	methyl acetate	-4.03	-6.67	-7.11
octane	CCCCCCCC	methyl acetate	-4.58	-7.39	-7.87
nonane	CCCCCCCCC	methyl acetate	-5.31	-8.56	-9.04
undecane	CCCCCCCCCCC	methyl acetate	-6.52	-10.53	-10.86
dodecane	CCCCCCCCCCCC	methyl acetate	-7.18	-11.38	-11.86
tetradecane	CCCCCCCCCCCCC	methyl acetate	-8.49	-13.43	-13.91
pentadecane	CCCCCCCCCCCCC	methyl acetate	-9.18	-14.04	-15.00
hexadecane	CCCCCCCCCCCCC	methyl acetate	-9.88	-15.75	-16.08
heptadecane	CCCCCCCCCCCCC	methyl acetate	-10.26	-16.96	-16.60
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	methyl acetate	-3.76	-6.50	-6.57
trichloromethane	ClC(Cl)Cl	methyl acetate	-4.24	-8.56	-7.69
1-chlorobutane	CCCCl	methyl acetate	-4.01	-7.60	-7.39
2-chlorobutane	CCC(C)Cl	methyl acetate	-3.85	-7.09	-7.11
1-chlorohexane	CCCCCCl	methyl acetate	-5.37	-9.32	-9.49
1-chloroheptane	CCCCCCCCl	methyl acetate	-6.00	-10.11	-10.44
1-chlorooctane	CCCCCCCCCl	methyl acetate	-6.60	-11.17	-11.30
1,3-dichloropropane	ClCCCl	methyl acetate	-5.12	-9.72	-9.08
1,4-dichlorobutane	ClCCCCl	methyl acetate	-6.02	-11.03	-10.47
1,5-dichloropentane	ClCCCCCl	methyl acetate	-6.74	-11.90	-11.66
1,6-dichlorohexane	ClCCCCCl	methyl acetate	-7.33	-13.01	-12.56
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	methyl acetate	-6.97	-12.99	-12.17
methyl chloroethanoate	COC(=O)CCl	methyl acetate	-6.15	-11.30	-11.30
1,2-dibromoethane	BrCCBr	methyl acetate	-5.50	-9.85	-9.83
1,4-dibromobutane	BrCCCCBr	methyl acetate	-6.94	-12.20	-12.12
1,5-dibromopentane	BrCCCCBr	methyl acetate	-7.47	-13.03	-12.98
1,6-dibromohexane	BrCCCCBr	methyl acetate	-7.94	-14.15	-13.70
butan-1-ol	CCCCO	methyl acetate	-5.42	-10.51	-10.84
2-butanol	CCC(C)O	methyl acetate	-5.11	-9.35	-10.26
<i>tert</i> -butanol	CC(C)(C)O	methyl acetate	-4.41	-9.65	-9.09
hexan-1-ol	CCCCCO	methyl acetate	-6.61	-12.19	-12.62
octan-1-ol	CCCCCCCCO	methyl acetate	-8.10	-14.10	-14.96
decan-1-ol	CCCCCCCCCO	methyl acetate	-9.09	-16.14	-16.30
methyl butanoate	CCCC(=O)OC	methyl acetate	-5.40	-9.38	-9.73
methyl pentanoate	CCCCC(=O)OC	methyl acetate	-5.98	-10.07	-10.56
methyl acetate	COC(C)=O	methyl acetate	-4.25	-7.72	-8.03
benzene	c1ccccc1	methyl acetate	-4.38	-7.67	-7.72
propylbenzene	CCc1ccccc1	methyl acetate	-6.22	-9.89	-10.46
dimethyl carbonate	COC(=O)OC	methyl acetate	-5.05	-9.08	-9.40
diethyl carbonate	CCOC(=O)OCC	methyl acetate	-5.67	-10.31	-10.15
acetic acid	CC(O)=O	methyl acetate	-6.14	-11.98	-12.88
<i>n</i> -methylpyrrole	Cn1cccc1	methyl acetate	-5.40	-9.71	-9.43
pyrrole	[nH]1cccc1	methyl acetate	-6.25	-11.63	-11.29
benzophenone	O=C(c1ccccc1)c2ccccc2	methyl acetate	-11.55	-17.73	-19.02
propylene carbonate	CC1COC(=O)O1	methyl acetate	-6.93	-14.64	-12.62

anthracene	c1ccc2cc3ccccc3cc2c1	methyl acetate		-10.88	-18.59	-17.99
pentane	CCCCC	methyl ethyl ketone		-2.72	-5.32	-5.39
hexane	CCCCCC	methyl ethyl ketone		-3.36	-6.35	-6.37
heptane	CCCCCCC	methyl ethyl ketone		-4.04	-7.45	-7.48
octane	CCCCCCCC	methyl ethyl ketone		-4.77	-8.43	-8.74
decane	CCCCCCCCC	methyl ethyl ketone		-6.00	-10.50	-10.55
cyclohexane	C1CCCCC1	methyl ethyl ketone		-3.62	-6.74	-6.30
methylcyclohexane	CC1CCCCC1	methyl ethyl ketone		-4.01	-7.31	-6.84
1-hexene	CCCCC=C	methyl ethyl ketone		-3.66	-8.04	-6.80
1-octene	CCCCCCC=C	methyl ethyl ketone		-5.02	-8.61	-8.96
cyclohexene	C1CCC=CC1	methyl ethyl ketone		-4.08	-7.28	-7.21
chloroform	ClC(Cl)Cl	methyl ethyl ketone		-4.36	-9.06	-7.89
tetrachloromethane	ClC(Cl)(Cl)Cl	methyl ethyl ketone		-4.39	-7.99	-7.99
1-chlorobutane	CCCCCl	methyl ethyl ketone		-4.03	-7.85	-7.37
1,1,2,3,3,3-hexafluoro-1-methoxypropane	COC(F)(F)C(F)C(F)(F)F	methyl ethyl ketone		-4.03	-8.68	-9.26
1,1,2,2-tetrafluoro-1-(2,2,2-trifluoroethoxy)ethane	FC(F)C(F)(F)OCC(F)(F)F	methyl ethyl ketone		-3.91	-9.78	-9.55
1,2-dimethoxyethane	COCCOC	methyl ethyl ketone		-4.89	-8.94	-8.40
1,4-dioxane	C1COCCO1	methyl ethyl ketone		-4.68	-6.74	-7.86
methanol	CO	methyl ethyl ketone		-3.95	-8.13	-8.72
ethanol	CCO	methyl ethyl ketone		-4.43	-8.68	-9.51
1-propanol	CCCO	methyl ethyl ketone		-5.09	-9.92	-10.52
1-butanol	CCCCO	methyl ethyl ketone		-5.68	-10.85	-11.43
1-hexanol	CCCCCO	methyl ethyl ketone		-7.02	-12.84	-13.44
2-butanol	CCC(C)O	methyl ethyl ketone		-5.26	-10.22	-10.63
isobutanol	CC(C)CO	methyl ethyl ketone		-5.64	-10.85	-11.40
2-methyl-isopropanol	CC(C)(C)O	methyl ethyl ketone		-4.51	-9.62	-9.37
acetone	CC(C)=O	methyl ethyl ketone		-3.68	-7.29	-6.68
butanone	CCC(C)=O	methyl ethyl ketone		-4.29	-8.32	-7.58
2-pentanone	CCCC(C)=O	methyl ethyl ketone		-4.86	-9.18	-8.49
2-heptanone	CCCCCC(C)=O	methyl ethyl ketone		-6.10	-11.16	-10.39
2-undecanone	CCCCCCCCC(C)=O	methyl ethyl ketone		-8.34	-15.60	-13.80
cyclohexanone	O=C1CCCCC1	methyl ethyl ketone		-6.45	-10.72	-11.17
acetonitrile	CC#N	methyl ethyl ketone		-4.77	-7.99	-7.77
propionitrile	CCC#N	methyl ethyl ketone		-5.22	-8.60	-8.36
butyronitrile	CCCC#N	methyl ethyl ketone		-5.61	-9.39	-8.86
acrylonitrile	C=CC#N	methyl ethyl ketone		-5.47	-7.81	-8.81
benzene	c1ccccc1	methyl ethyl ketone		-4.21	-8.14	-7.40
ethylbenzene	CCc1ccccc1	methyl ethyl ketone		-5.49	-10.02	-9.40
1,4-dimethylbenzene	Cc1ccc(C)cc1	methyl ethyl ketone		-5.45	-10.03	-9.41
1,2,4-trimethylbenzene	Cc1ccc(C)c(C)c1	methyl ethyl ketone		-6.02	-11.25	-10.33
chlorobenzene	Clc1ccccc1	methyl ethyl ketone		-5.39	-10.02	-9.20
n-methylpyrrole	Cn1cccc1	methyl ethyl ketone		-5.26	-9.73	-9.16
N-methylimidazole	Cn1ccnc1	methyl ethyl ketone		-7.17	-12.75	-12.01
dimethyl carbonate	COC(=O)OC	methyl ethyl ketone		-4.51	-8.84	-7.58
diethyl carbonate	CCOC(=O)OCC	methyl ethyl ketone		-4.96	-10.36	-8.22
dimethyl sulfoxide	C[S](C)=O	methyl ethyl ketone		-6.91	-12.25	-11.88
anthracene	c1ccc2cc3ccccc3cc2c1	methyl ethyl ketone		-10.82	-16.39	-17.86
anthraquinone	O=C1c2ccccc2C(=O)c3ccccc13	methyl ethyl ketone		-14.13	-22.76	-23.24
pentane	CCCCC	nitromethane		-1.89	-3.54	-3.83
heptane	CCCCCCC	nitromethane		-3.02	-4.96	-5.60
octane	CCCCCCCC	nitromethane		-3.46	-6.50	-6.29
2,3-dimethylbutane	CC(C)C(C)C	nitromethane		-2.02	-3.90	-4.02
cyclohexane	C1CCCCC1	nitromethane		-2.78	-4.64	-4.77
chloroform	ClC(Cl)Cl	nitromethane		-4.09	-7.17	-7.59
tetrachloromethane	ClC(Cl)(Cl)Cl	nitromethane		-4.25	-6.38	-8.01
1-chlorobutane	CCCCCl	nitromethane		-3.91	-6.42	-7.30
methanol	CO	nitromethane		-3.53	-6.67	-8.05
ethanol	CCO	nitromethane		-3.94	-7.26	-8.70
1-butanol	CCCCO	nitromethane		-4.93	-8.79	-10.26
1-pentanol	CCCCCO	nitromethane		-5.24	-9.54	-10.65
1-hexanol	CCCCCO	nitromethane		-6.35	-10.22	-12.53
nitromethane	C[N+](=O)[O-]	nitromethane		-4.84	-9.15	-9.37
1-nitropropane	CCC[N+](=O)[O-]	nitromethane		-5.95	-10.02	-10.85
acetonitrile	CC#N	nitromethane		-4.29	-7.87	-6.78
propionitrile	CCC#N	nitromethane		-5.00	-8.41	-7.96
butyronitrile	CCCC#N	nitromethane		-5.53	-8.94	-8.81
ethylbenzene	CCc1ccccc1	nitromethane		-5.20	-8.51	-8.99
pyrrole	[nH]1cccc1	nitromethane		-5.68	-10.45	-10.34
n-methylpyrrole	Cn1cccc1	nitromethane		-4.78	-9.11	-8.59
water	O	nitromethane		-4.18	-7.17	-10.24
1-bromoadamantane	BrC12CC3CC(C(C3)C1)C2	nitromethane		-7.23	-11.35	-11.38
1-adamantanol	OC12CC3CC(C(C3)C1)C2	nitromethane		-9.20	-12.91	-15.92
2-adamantanone	O=C1C2CC3CC(C2)CC1C3	nitromethane		-9.43	-16.42	-15.29
N-methylimidazole	Cn1ccnc1	nitromethane		-6.97	-13.39	-11.79
imidazole	[nH]1ccnc1	nitromethane		-8.56	-14.99	-15.26
carbon dioxide	O=C=O	N-methyl-2-pyrrolidone		-0.48	-3.56	-3.06
COS	O=C=S	N-methyl-2-pyrrolidone		-1.70	-3.61	-4.03
methane	C	N-methyl-2-pyrrolidone		0.46	-0.53	-1.23
propane	CCC	N-methyl-2-pyrrolidone		-0.76	-3.03	-2.92
pentane	CCCCC	N-methyl-2-pyrrolidone		-1.85	-4.47	-4.52
heptane	CCCCCCC	N-methyl-2-pyrrolidone		-3.01	-7.07	-6.36

2-methylbutane	CCC(C)C	N-methyl-2-pyrrolidone	-1.69	-4.30	-4.27
2,2-dimethylbutane	CCC(C)(C)C	N-methyl-2-pyrrolidone	-2.03	-4.57	-4.94
2,2-dimethylpentane	CCCC(C)(C)C	N-methyl-2-pyrrolidone	-2.54	-5.19	-5.76
2,4-dimethylpentane	CC(C)CC(C)C	N-methyl-2-pyrrolidone	-2.51	-6.11	-5.55
2,2,3-trimethylbutane	CC(C)C(C)(C)C	N-methyl-2-pyrrolidone	-2.43	-5.97	-5.67
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	N-methyl-2-pyrrolidone	-2.90	-5.94	-6.45
cyclopentane	C1CCCC1	N-methyl-2-pyrrolidone	-2.68	-5.40	-5.84
methylcyclopentane	CC1CCCC1	N-methyl-2-pyrrolidone	-3.02	-6.24	-6.28
cyclohexane	C1CCCCC1	N-methyl-2-pyrrolidone	-3.19	-6.34	-6.57
methylcyclohexane	CC1CCCCC1	N-methyl-2-pyrrolidone	-3.41	-7.23	-6.83
1-pentene	CCCC=C	N-methyl-2-pyrrolidone	-2.29	-4.24	-5.13
1-hexene	CCCCC=C	N-methyl-2-pyrrolidone	-2.90	-5.79	-6.11
1-heptene	CCCCC=C	N-methyl-2-pyrrolidone	-3.45	-7.75	-6.97
1-octene	CCCCC=C	N-methyl-2-pyrrolidone	-4.04	-7.87	-7.92
1,3-pentadiene	CC=CC=C	N-methyl-2-pyrrolidone	-2.79	-6.06	-5.90
1,3-cyclohexadiene	C1CC=CC=C1	N-methyl-2-pyrrolidone	-3.75	-6.15	-7.31
methanol	CO	N-methyl-2-pyrrolidone	-3.65	-9.48	-9.02
ethanol	CCO	N-methyl-2-pyrrolidone	-4.18	-9.37	-9.97
isopropanol	CC(C)O	N-methyl-2-pyrrolidone	-4.42	-10.16	-10.43
2-methyl-isopropanol	CC(C)(C)O	N-methyl-2-pyrrolidone	-4.47	-11.08	-10.53
1,2-ethanediol	OCCO	N-methyl-2-pyrrolidone	-6.19	-16.42	-15.12
1,3-butanediol	CC(O)CCO	N-methyl-2-pyrrolidone	-7.55	-17.95	-17.32
1,4-butanediol	OCCCCO	N-methyl-2-pyrrolidone	-8.55	-19.60	-18.76
1-chlorobutane	CCCCCl	N-methyl-2-pyrrolidone	-3.79	-8.18	-7.65
1-chlorooctane	CCCCCCCCCl	N-methyl-2-pyrrolidone	-6.11	-11.68	-11.41
1,2-dichloroethane	ClCCCl	N-methyl-2-pyrrolidone	-4.02	-9.57	-7.71
1,4-dichlorobutane	ClCCCCCl	N-methyl-2-pyrrolidone	-5.85	-11.63	-10.51
1,6-dichlorohexane	ClCCCCCCCCl	N-methyl-2-pyrrolidone	-7.58	-13.56	-13.42
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	N-methyl-2-pyrrolidone	-5.26	-8.26	-9.88
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	N-methyl-2-pyrrolidone	-6.78	-14.48	-12.39
trichloroethene	ClC=C(Cl)Cl	N-methyl-2-pyrrolidone	-4.27	-9.48	-8.58
tetrachloroethene	ClC(Cl)=C(Cl)Cl	N-methyl-2-pyrrolidone	-4.22	-9.55	-8.60
iodoethane	CCl	N-methyl-2-pyrrolidone	-3.91	-7.45	-7.68
butyraldehyde	CCCC=O	N-methyl-2-pyrrolidone	-4.01	-7.62	-7.76
isobutyraldehyde	CC(C)C=O	N-methyl-2-pyrrolidone	-3.97	-6.93	-7.75
pentanal	CCCCC=O	N-methyl-2-pyrrolidone	-4.44	-7.95	-8.30
crotonaldehyde	C/C=C/O	N-methyl-2-pyrrolidone	-4.19	-8.71	-7.91
methyl ethyl ketone	CCC(C)=O	N-methyl-2-pyrrolidone	-4.02	-8.43	-7.74
methyl isobutyl ketone	CC(C)CC(C)=O	N-methyl-2-pyrrolidone	-4.94	-10.05	-9.29
cyclohexanone	O=C1CCCCC1	N-methyl-2-pyrrolidone	-5.82	-10.71	-10.73
acetophenone	CC(=O)c1ccccc1	N-methyl-2-pyrrolidone	-7.24	-13.97	-12.48
methyl acetate	COC(C)=O	N-methyl-2-pyrrolidone	-4.02	-7.31	-7.72
propyl acetate	CCCOC(C)=O	N-methyl-2-pyrrolidone	-4.75	-8.69	-9.04
vinyl acetate	CC(=O)OC=C	N-methyl-2-pyrrolidone	-4.58	-7.92	-8.54
toluene	Cc1ccccc1	N-methyl-2-pyrrolidone	-4.45	-9.21	-8.44
naphthalene	c1ccc2ccccc2c1	N-methyl-2-pyrrolidone	-6.99	-14.16	-12.43
biphenyl	c1ccc(cc1)c2ccccc2	N-methyl-2-pyrrolidone	-8.57	-16.31	-14.66
phenanthrene	c1ccc2c(c1)ccc3ccccc23	N-methyl-2-pyrrolidone	-10.67	-20.00	-18.33
p-terphenyl	c1ccc(cc1)c2ccc(cc2)c3ccccc3	N-methyl-2-pyrrolidone	-13.42	-25.00	-21.93
phenol	Oc1ccccc1	N-methyl-2-pyrrolidone	-7.55	-18.31	-14.83
4-chlorophenol	Oc1ccc(Cl)cc1	N-methyl-2-pyrrolidone	-9.23	-20.87	-17.53
thiophene	s1ccccc1	N-methyl-2-pyrrolidone	-4.71	-7.76	-9.08
3-nitrophenol	Oc1cccc(c1)[N+](=O)[O-]	N-methyl-2-pyrrolidone	-11.49	-24.14	-21.39
4-nitrophenol	Oc1ccc(cc1)[N+](=O)[O-]	N-methyl-2-pyrrolidone	-11.52	-25.26	-21.38
4-fluorophenol	Oc1ccc(F)cc1	N-methyl-2-pyrrolidone	-8.26	-17.91	-16.48
4-fluoroanisole	COc1ccc(F)cc1	N-methyl-2-pyrrolidone	-6.71	-12.14	-12.46
N-methyl-2-pyrrolidone	CN1CCCC1=O	N-methyl-2-pyrrolidone	-7.64	-13.12	-14.62
water	O	N-methyl-2-pyrrolidone	-4.30	-11.70	-11.30
formamide	NC=O	N-methyl-2-pyrrolidone	-7.46	-16.30	-14.76
propiophenone	CCC(=O)c1ccccc1	N-methyl-2-pyrrolidone	-7.85		-13.45
hexane	CCCCCC	2-methoxyethanol	-2.76	-5.88	-5.69
heptane	CCCCCCC	2-methoxyethanol	-3.45	-6.86	-6.80
decane	CCCCCCCCC	2-methoxyethanol	-5.59	-9.70	-10.26
dodecane	CCCCCCCCCCC	2-methoxyethanol	-6.86	-11.76	-12.36
methylcyclohexane	CC1CCCCC1	2-methoxyethanol	-3.79	-6.79	-6.94
benzene	c1ccccc1	2-methoxyethanol	-3.83	-7.93	-7.22
o-xylene	Cc1ccccc1C	2-methoxyethanol	-5.20	-9.78	-9.43
m-xylene	Cc1ccc(C)cc1	2-methoxyethanol	-5.22	-9.66	-9.43
p-xylene	Cc1cc(C)cc1	2-methoxyethanol	-5.22	-9.63	-9.43
fluorobenzene	Fc1ccccc1	2-methoxyethanol	-4.27	-8.58	-8.05
chlorobenzene	Clc1ccccc1	2-methoxyethanol	-5.36	-9.87	-9.68
bromobenzene	Brc1ccccc1	2-methoxyethanol	-5.87	-10.64	-10.59
naphthalene	c1ccc2ccccc2c1	2-methoxyethanol	-7.46	-13.29	-12.98
biphenyl	c1ccc(cc1)c2ccccc2	2-methoxyethanol	-8.91	-15.34	-14.95
2-chloro-2-methylpropane	CC(C)(C)Cl	2-methoxyethanol	-3.36	-6.41	-6.70
heptane	CCCCCC	propylene glycol	-2.89	-7.19	-6.83
nonane	CCCCCCCC	propylene glycol	-4.34	-9.20	-9.24
cyclohexane	C1CCCCC1	propylene glycol	-2.89	-6.81	-6.60
benzene	c1ccccc1	propylene glycol	-3.51	-7.39	-7.50
toluene	Cc1ccccc1	propylene glycol	-4.10	-8.25	-8.40
ethylbenzene	CCc1ccccc1	propylene glycol	-4.66	-9.20	-9.22
m-xylene	Cc1ccc(C)cc1	propylene glycol	-4.63	-9.20	-9.23
p-xylene	Cc1cc(C)cc1	propylene glycol	-4.64	-9.15	-9.24

fluorobenzene	Fc1ccccc1	propylene glycol		-4.01	-7.86	-8.41
chlorobenzene	Clc1ccccc1	propylene glycol		-5.00	-9.15	-9.86
bromobenzene	Brc1ccccc1	propylene glycol		-5.43	-9.82	-10.54
naphthalene	c1ccc2ccccc2c1	propylene glycol		-6.90	-12.17	-12.88
1,2-propylene glycol	CC(O)CO	propylene glycol		-6.65	-16.13	-16.13
methanol	CO	propylene glycol		-3.48	-8.99	-9.44
ethanol	CCO	propylene glycol		-3.96	-9.95	-10.27
1,4-dioxane	C1COCCO1	cyclohexanone		-4.85	-9.01	-8.67
cyclohexanone	O=C1CCCCC1	cyclohexanone		-6.26	-10.77	-10.96
benzene	c1ccccc1	cyclohexanone		-4.05	-8.34	-7.39
ethylbenzene	CCc1ccccc1	cyclohexanone		-5.42	-10.17	-9.58
isopropylbenzene	CC(C)c1ccccc1	cyclohexanone		-6.11	-10.82	-10.74
<i>n</i> -methylpyrrole	Cn1cccc1	cyclohexanone		-5.32	-9.83	-9.91
pyrrole	[nH]1cccc1	cyclohexanone		-6.09	-12.22	-11.14
anthracene	c1ccc2cc3ccccc3cc2c1	cyclohexanone		-10.83	-19.22	-18.00
helium	[He]	cyclohexanone		2.10	2.58	2.18
krypton	[Kr]	cyclohexanone		0.47	-0.81	-0.44
xenon	[Xe]	cyclohexanone		-0.49	-2.03	-2.11
hydrogen	[H][H]	cyclohexanone		1.59	1.38	1.13
deuterium	[H][H]	cyclohexanone		1.59	1.30	1.13
nitrogen	N#N	cyclohexanone		1.01	0.65	0.34
oxygen	O=O	cyclohexanone		0.99	0.26	-0.10
ethene	C=C	cyclohexanone		-0.80	-2.28	-2.55
ethane	CC	cyclohexanone		-0.36	-2.33	-1.90
tetrafluoromethane	FC(F)(F)F	cyclohexanone		1.10	0.31	-0.07
sulfur hexafluoride	F[S](F)(F)(F)(F)F	cyclohexanone		0.56	-0.98	-0.85
carbon dioxide	O=C=O	cyclohexanone		-0.55	-3.35	-2.67
heptane	CCCCCCC	cyclohexanone		-3.86	-7.49	-7.54
nonane	CCCCCCCCC	cyclohexanone		-5.28	-9.80	-9.87
cyclohexane	C1CCCCC1	cyclohexanone		-3.53	-7.12	-6.51
methylcyclohexane	CC1CCCCC1	cyclohexanone		-4.07	-7.59	-7.38
1,2-dimethoxyethane	COCCOC	cyclohexanone		-5.08	-8.77	-9.31
4-fluorophenol	Oc1ccc(F)cc1	cyclohexanone		-8.33	-14.11	-16.09
dimethyl carbonate	COC(=O)OC	cyclohexanone		-4.38	-8.63	-7.73
propylene carbonate	CC1COC(=O)O1	cyclohexanone		-6.24	-14.46	-11.15
15-crown-5	C1COCCOCCOCCOCCO1	cyclohexanone		-10.49	-18.80	-20.11
1-hexene	CCCCC=C	methylcyclohexane		-3.92	-7.24	-7.19
helium	[He]	2-methyltetrahydrofuran		2.10	1.02	2.22
krypton	[Kr]	2-methyltetrahydrofuran		0.06	-1.04	-0.65
xenon	[Xe]	2-methyltetrahydrofuran		-0.96	-1.56	-2.29
deuterium	[H][H]	2-methyltetrahydrofuran		1.30	0.53	0.84
methane	C	2-methyltetrahydrofuran		0.05	-0.90	-0.97
ethene	C=C	2-methyltetrahydrofuran		-1.55	-1.70	-3.75
ethane	CC	2-methyltetrahydrofuran		-0.90	-1.79	-2.48
sulfur hexafluoride	F[S](F)(F)(F)(F)F	2-methyltetrahydrofuran		0.36	-1.24	-0.81
hexane	CCCCCC	2-methyltetrahydrofuran		-3.83	-7.00	-7.14
heptane	CCCCCCC	2-methyltetrahydrofuran		-4.51	-8.15	-8.20
octane	CCCCCCCC	2-methyltetrahydrofuran		-5.10	-9.27	-9.07
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	2-methyltetrahydrofuran		-4.25	-7.86	-7.69
decane	CCCCCCCCC	2-methyltetrahydrofuran		-6.53	-11.47	-11.35
undecane	CCCCCCCCCCC	2-methyltetrahydrofuran		-7.05	-12.55	-12.08
dodecane	CCCCCCCCCCCC	2-methyltetrahydrofuran		-7.72	-13.72	-13.10
hexadecane	CCCCCCCCCCCCCCC	2-methyltetrahydrofuran		-10.25	-18.18	-17.03
cyclohexane	C1CCCCC1	2-methyltetrahydrofuran		-4.03	-7.48	-6.99
methylcyclohexane	CC1CCCCC1	2-methyltetrahydrofuran		-4.56	-8.03	-7.81
cyclooctane	C1CCCCCCC1	2-methyltetrahydrofuran		-5.40	-10.28	-9.12
methylcyclopentane	CC1CCCC1	2-methyltetrahydrofuran		-3.85	-7.22	-6.68
1-hexene	CCCCC=C	2-methyltetrahydrofuran		-4.27	-7.12	-7.98
1-chlorobutane	CCCCCl	2-methyltetrahydrofuran		-4.31	-8.24	-7.97
2-chlorobutane	CCC(C)Cl	2-methyltetrahydrofuran		-4.16	-7.69	-7.69
2-methyl-1-chloropropane	CC(C)CCl	2-methyltetrahydrofuran		-4.16	-7.81	-7.70
2-methyl-2-chloropropane	CC(C)(C)Cl	2-methyltetrahydrofuran		-3.85	-7.06	-7.21
chlorocyclohexane	ClC1CCCCC1	2-methyltetrahydrofuran		-5.77	-10.27	-9.85
methyl <i>tert</i> -butyl ether	COC(C)(C)C	2-methyltetrahydrofuran		-3.56	-7.08	-6.41
2-methyltetrahydrofuran	CC1CCCO1	2-methyltetrahydrofuran		-4.31	-8.27	-7.28
fluorobenzene	Fc1ccccc1	2-methyltetrahydrofuran		-4.83	-8.84	-8.63
methanol	CO	2-methyltetrahydrofuran		-3.91	-8.46	-8.61
ethanol	CCO	2-methyltetrahydrofuran		-4.59	-9.27	-9.75
1-propanol	CCCO	2-methyltetrahydrofuran		-5.30	-10.52	-10.88
1-butanol	CCCCO	2-methyltetrahydrofuran		-5.89	-11.69	-11.77
2-butanol	CCC(C)O	2-methyltetrahydrofuran		-5.44	-10.95	-10.89
isobutanol	CC(C)CO	2-methyltetrahydrofuran		-5.79	-11.47	-11.60
2-methyl-isopropanol	CC(C)(C)O	2-methyltetrahydrofuran		-4.74	-9.92	-9.71
1-pentanol	CCCCCO	2-methyltetrahydrofuran		-6.31	-12.76	-12.26
helium	[He]	fluorobenzene	2.07	1.82		1.97
neon	[Ne]	fluorobenzene	1.91	2.00		2.06
argon	[Ar]	fluorobenzene	0.72	0.72		0.27
krypton	[Kr]	fluorobenzene	0.08	-0.10		-0.79
xenon	[Xe]	fluorobenzene	-0.72	-1.07		-2.10
oxygen	O=O	fluorobenzene	0.56	0.25		-0.82
octane	CCCCCCCC	fluorobenzene	-5.16	-5.19		-8.96
1,4-dioxane	C1COCCO1	fluorobenzene	-5.16	-5.51		-9.54
methyl ethyl ketone	CCC(C)=O	fluorobenzene	-4.64	-5.24		-9.64



nitromethane	C[N+](=[O-])=O	fluorobenzene	-4.47	-5.37		-10.44
ethanol	CCO	fluorobenzene	-3.25	-4.72		-9.85
toluene	Cc1ccccc1	fluorobenzene	-5.22	-5.73		-10.03
fluorobenzene	Fc1ccccc1	fluorobenzene	-4.64	-5.47		-9.89
trifluoromethane	FC(F)F	fluorobenzene	-0.49	-1.12		-2.40
helium	[He]	chlorobenzene	2.43	1.98	2.40	1.95
neon	[Ne]	chlorobenzene	2.22	1.84	2.30	1.65
xenon	[Xe]	chlorobenzene	-0.64	-0.79	-2.08	-2.25
radon	[Rn]	chlorobenzene	-1.50	-0.96		-2.44
hydrogen	[H][H]	chlorobenzene	1.65	1.63	1.19	1.32
deuterium	[H][H]	chlorobenzene	1.65	1.63		1.32
oxygen	O=O	chlorobenzene	1.00	0.66	0.15	-0.20
nitrogen	N#N	chlorobenzene	1.35	0.94	0.58	0.69
nitrous oxide	[O-][N+]=[N]	chlorobenzene	-0.68	-0.90		-2.08
ammonia	N	chlorobenzene	-1.36	-2.20	-3.56	-4.33
carbon dioxide	O=C=O	chlorobenzene	-0.50	-0.91		-2.94
iodine	I2	chlorobenzene	-5.81	-5.86	-9.61	-9.65
hydrogen sulfide	S	chlorobenzene	-1.50	-1.91	-2.89	-3.09
methane	C	chlorobenzene	0.45	0.11	-0.61	-0.84
propane	CCC	chlorobenzene	-1.61	-1.32	-3.77	-2.97
butane	CCCC	chlorobenzene	-2.32	-1.95		-3.94
isobutane	CC(C)C	chlorobenzene	-2.25	-1.90		-3.90
pentane	CCCCC	chlorobenzene	-3.31	-2.61		-4.99
hexane	CCCCCC	chlorobenzene	-4.02	-3.37		-6.22
heptane	CCCCCCC	chlorobenzene	-4.73	-4.10		-7.40
octane	CCCCCCCC	chlorobenzene	-5.44	-4.73		-8.47
nonane	CCCCCCCCC	chlorobenzene	-6.17	-5.54		-9.75
2-methylpentane	CCCC(C)C	chlorobenzene	-3.79	-3.19		-5.92
2,5-dimethylhexane	CC(C)CCC(C)C	chlorobenzene	-4.97	-4.46		-7.98
2,3,4-trimethylpentane	CC(C)(C)C(C)C	chlorobenzene	-5.03	-4.10		-7.42
cyclohexane	C1CCCCC1	chlorobenzene	-4.41	-4.10	-7.31	-7.27
ethylcyclohexane	CCC1CCCCC1	chlorobenzene	-5.54	-5.40		-9.36
ethene	C=C	chlorobenzene	-0.61	-0.89		-2.26
tetrafluoromethane	FC(F)(F)F	chlorobenzene	1.30	1.02		0.19
difluoromethane	FCF	chlorobenzene	-0.84	-1.58		-3.32
trifluoromethane	FC(F)F	chlorobenzene	0.08	-0.86		-2.24
chloromethane	CCl	chlorobenzene	-2.21	-2.00		-4.09
chloroethane	CCCl	chlorobenzene	-2.96	-2.91		-5.57
tert-butyl chloride	CC(C)(C)Cl	chlorobenzene	-3.56	-4.16		-7.60
1-chlorobutane	CCCCCl	chlorobenzene	-4.35	-4.64		-8.44
bromoethane	CCBr	chlorobenzene	-3.51	-3.48		-6.63
iodoethane	CCl	chlorobenzene	-4.17	-4.44		-7.68
dimethyl ether	COC	chlorobenzene	-2.18	-2.68		-5.17
1,4-dioxane	O1CCOCC1	chlorobenzene	-5.07	-5.23	-9.35	-9.18
propanone	CC(C)=O	chlorobenzene	-3.63	-4.17		-7.62
ethyl acetate	CCOC(C)=O	chlorobenzene	-4.43	-4.91	-8.55	-8.70
triethylamine	CCN(CC)CC	chlorobenzene	-4.57	-4.74	-8.52	-9.35
acetonitrile	CC#N	chlorobenzene	-3.74	-4.65	-7.33	-7.52
propionitrile	CCC#N	chlorobenzene	-4.45	-5.36	-8.60	-8.70
methanol	CO	chlorobenzene	-2.28	-3.04	-6.25	-6.49
1-propanol	CCCO	chlorobenzene	-3.83	-4.35		-8.76
2-butanol	CCC(C)O	chlorobenzene	-4.26	-4.79		-9.50
1-pentanol	CCCCCO	chlorobenzene	-5.48	-5.65		-10.91
isobutanol	CC(C)CO	chlorobenzene	-4.26	-4.96		-9.76
3-methyl-1-butanol	CC(C)CCO	chlorobenzene	-5.13	-5.65		-10.83
2-chloroethanol	OCCCl	chlorobenzene	-4.62	-6.10		-11.33
1,3-dichloro-isopropanol	OC(CCl)CCl	chlorobenzene	-6.02	-8.22		-14.42
sulfur hexafluoride	F[S](F)(F)(F)(F)F	chlorobenzene	0.35	0.34		-1.19
tetramethylstannane	C[Sn](C)(C)C	chlorobenzene	-4.04	-3.86	-7.34	-6.56
tetraethyltin	CC[Sn](CC)(CC)CC	chlorobenzene	-7.23	-6.02		-9.93
benzene	c1ccccc1	chlorobenzene	-4.42	-4.61	-8.08	-8.28
toluene	Cc1ccccc1	chlorobenzene	-5.21	-5.35	-9.19	-9.46
chlorobenzene	Clc1ccccc1	chlorobenzene	-5.70	-5.98	-9.80	-10.36
ammonia	N	chlorobenzene	-1.28	-2.20	-3.56	-4.33
diethyl ether	CCOCC	chlorobenzene	-4.04	-3.93	-6.90	-7.22
tetrahydrofuran	C1CCOC1	chlorobenzene	-4.05	-4.51	-8.30	-8.08
2-propanone	CC(C)=O	chlorobenzene	-3.87	-4.17		-7.62
2-pentanone	CCCC(C)=O	chlorobenzene	-5.28	-5.44		-9.62
2-hexanone	CCCCC(C)=O	chlorobenzene	-5.84	-6.13		-10.74
2-heptanone	CCCCCC(C)=O	chlorobenzene	-6.47	-6.87		-11.97
tert-butyl methyl ketone	CC(=O)C(C)C	chlorobenzene	-5.47	-5.42		-9.63
acetylacetone	CC(=O)CC(C)=O	chlorobenzene	-5.87	-6.82		-11.57
4,6-nonanedione	CCCC(=O)CC(=O)CCC	chlorobenzene	-8.23	-9.18		-15.57
methyl acetate	COC(C)=O	chlorobenzene	-3.82	-4.55	-7.68	-8.10
ethyl acetate	CCOC(C)=O	chlorobenzene	-4.47	-4.91	-8.55	-8.70
propyl acetate	CCCOC(C)=O	chlorobenzene	-5.09	-5.40	-9.31	-9.55
butyl acetate	CCCCOC(C)=O	chlorobenzene	-5.84	-6.02	-10.59	-10.60
methyl propanoate	CCC(=O)OC	chlorobenzene	-4.56	-4.80		-8.46
methylamine	CN	chlorobenzene	-2.16	-2.63		-5.24
propylamine	CCCN	chlorobenzene	-3.59	-3.97		-7.92
butylamine	CCCCN	chlorobenzene	-4.17	-4.67		-9.19
dimethylamine	CNC	chlorobenzene	-2.76	-3.25		-6.71
trimethylamine	CN(C)C	chlorobenzene	-2.80	-3.09		-6.24

triethylamine	CCN(CC)CC	chlorobenzene	-4.67	-4.74	-8.52	-9.35
propanoic acid	CCC(O)=O	chlorobenzene	-4.37	-5.71		-11.04
methacrylic acid	CC(=C)C(O)=O	chlorobenzene	-5.37	-5.88		-11.05
ethanol	CCO	chlorobenzene	-2.69	-3.65	-7.27	-7.58
1-propanol	CCCO	chlorobenzene	-3.85	-4.35		-8.76
1-butanol	CCCCO	chlorobenzene	-4.31	-5.06		-9.97
1-pentanol	CCCCCO	chlorobenzene	-5.35	-5.65		-10.91
1-hexanol	CCCCCCO	chlorobenzene	-6.03	-6.57		-12.36
2-ethoxyethanol	CCOCCO	chlorobenzene	-4.92	-6.44		-12.54
2-isopropoxyethanol	CC(C)OCCO	chlorobenzene	-5.42	-6.55		-13.06
aniline	Nc1ccccc1	chlorobenzene	-7.09	-7.36	-12.62	-12.51
neon	[Ne]	bromobenzene	2.37	1.80		1.58
xenon	[Xe]	bromobenzene	-0.55	-0.64		-2.38
hydrogen	[H][H]	bromobenzene	1.77	1.69		1.31
deuterium	[H][H]	bromobenzene	1.76	1.69		1.31
oxygen	O=O	bromobenzene	1.16	0.65		-0.76
nitrogen	N#N	bromobenzene	1.54	0.97		0.29
carbon monoxide	[C-]#[O+]	bromobenzene	1.19	0.65		-0.50
methane	C	bromobenzene	0.57	0.41		-0.71
ethane	CC	bromobenzene	-0.61	-0.39		-1.90
propane	CCC	bromobenzene	-1.43	-1.09		-2.98
octane	CCCCCCCC	bromobenzene	-5.10	-4.54		-8.54
ethene	C=C	bromobenzene	-0.52	-0.63		-2.20
tetrafluoromethane	FC(F)(F)F	bromobenzene	1.57	1.30		0.30
fluoromethane	CF	bromobenzene	-0.73	-1.02		-2.97
difluoromethane	FCF	bromobenzene	-0.78	-1.32		-3.28
trifluoromethane	FC(F)F	bromobenzene	0.02	-0.59		-2.17
chloroethane	CCCl	bromobenzene	-2.17	-2.70		-5.61
tert-butyl chloride	CC(C)(C)Cl	bromobenzene	-3.44	-3.97		-7.68
tert-butyl bromide	CC(C)(C)Br	bromobenzene	-3.89	-4.10		-7.92
iodoethane	CCl	bromobenzene	-4.22	-4.16		-7.61
dimethyl ether	COC	bromobenzene	-2.10	-2.44		-5.16
1,4-dioxane	C1COCCO1	bromobenzene	-5.22	-4.98		-9.17
methyl ethyl ketone	CCC(C)=O	bromobenzene	-4.39	-4.55		-8.54
triethylamine	CCN(CC)CC	bromobenzene	-4.47	-4.47		-9.24
ethanol	CCO	bromobenzene	-3.06	-3.39		-7.51
1-propanol	CCCO	bromobenzene	-3.66	-4.12		-8.74
1-butanol	CCCCO	bromobenzene	-4.54	-4.83		-9.95
2-butanol	CCC(C)O	bromobenzene	-4.15	-4.56		-9.48
1-pentanol	CCCCCO	bromobenzene	-5.42	-5.42		-10.90
1-hexanol	CCCCCCO	bromobenzene	-5.98	-6.34		-12.35
isobutanol	CC(C)CO	bromobenzene	-4.23	-4.73		-9.75
3-methyl-1-butanol	CC(C)CCO	bromobenzene	-5.27	-5.42		-10.81
cyclohexanol	OC1CCCCC1	bromobenzene	-6.47	-6.94		-13.34
sulfur hexafluoride	F[S](F)(F)(F)(F)F	bromobenzene	0.67	0.57		-1.30
tetramethylstannane	C[Sn](C)(C)C	bromobenzene	-3.59	-3.75		-6.86
toluene	Cc1ccccc1	bromobenzene	-5.17	-5.11		-9.44
bromobenzene	Brc1ccccc1	bromobenzene	-6.30	-6.20		-11.11
tetrahydrofuran	O1CCCC1	bromobenzene	-3.96	-4.32		-8.17
acetylacetone	CC(=O)CC(C)=O	bromobenzene	-5.91	-6.70		-11.84
ethyl acetate	CCOC(C)=O	bromobenzene	-4.42	-4.61		-8.61
propyl acetate	CCCOC(C)=O	bromobenzene	-4.87	-5.19		-9.59
butyl acetate	CCCCOC(C)=O	bromobenzene	-5.67	-5.81		-10.64
pentyl acetate	CCCCCOC(C)=O	bromobenzene	-6.41	-6.49		-11.79
ethylamine	CCN	bromobenzene	-2.73	-3.10		-6.69
propylamine	CCCN	bromobenzene	-3.57	-3.75		-7.91
butylamine	CCCCN	bromobenzene	-4.15	-4.45		-9.18
methanol	CO	bromobenzene	-2.31	-2.78		-6.42
ethanol	CCO	bromobenzene	-2.69	-3.39		-7.51
1-propanol	CCCO	bromobenzene	-3.77	-4.12		-8.74
1-pentanol	CCCCCO	bromobenzene	-5.16	-5.42		-10.90
1-hexanol	CCCCCCO	bromobenzene	-5.96	-6.34		-12.35
ethoxyethanol	CCOC(C)O	bromobenzene	-4.92	-5.15		-10.86
isopropoxyethanol	CC(C)OC(C)O	bromobenzene	-5.42	-5.09		-10.52
o-cresol	Cc1ccccc1O	bromobenzene	-7.27	-7.61		-14.05
p-cresol	Cc1ccc(O)cc1	bromobenzene	-7.12	-7.65		-13.99
neon	[Ne]	iodobenzene	2.63	1.71		1.40
argon	[Ar]	iodobenzene	1.31	1.08		-0.04
krypton	[Kr]	iodobenzene	0.59	0.47		-1.12
xenon	[Xe]	iodobenzene	-0.40	-0.44		-2.58
oxygen	O=O	iodobenzene	1.30	0.73		-1.27
ethane	CC	iodobenzene	-0.61	-0.03		-1.82
octane	CCCCCCCC	iodobenzene	-4.76	-4.33		-8.74
chloromethane	CCl	iodobenzene	-2.10	-1.37		-3.98
iodoethane	CCl	iodobenzene	-4.28	-3.73		-7.43
dioxane	C1COCCO1	iodobenzene	-4.95	-4.53		-8.95
triethylamine	CCN(CC)CC	iodobenzene	-4.34	-4.06		-8.98
nitromethane	C[N+](=O)[O-]	iodobenzene	-4.00	-4.52		-9.62
ethanol	CCO	iodobenzene	-2.96	-2.96		-7.32
toluene	Cc1ccccc1	iodobenzene	-5.05	-4.74		-9.36
acetylacetone	CC(=O)CC(C)=O	iodobenzene	-5.91	-6.52		-12.29
ethanol	CCO	iodobenzene	-2.39	-2.96		-7.32
propan-1-ol	CCCO	iodobenzene	-3.55	-3.72		-8.56

pentan-1-ol	CCCCCO	iodobenzene	-5.12	-5.17		-10.99
hexan-1-ol	CCCCCCO	iodobenzene	-5.76	-5.79		-12.00
heptan-1-ol	CCCCCCCO	iodobenzene	-6.51	-6.58		-13.34
ethylamine	CCN	iodobenzene	-2.73	-2.71		-6.54
propylamine	CCCN	iodobenzene	-3.55	-3.37		-7.77
butylamine	CCCCN	iodobenzene	-4.08	-4.07		-9.05
acetylacetone	CC(=O)CC(C)=O	iodobenzene	-5.91	-6.52		-12.29
o-cresol	Cc1ccccc1O	iodobenzene	-7.15	-7.10		-13.69
m-cresol	Cc1cccc(O)c1	iodobenzene	-6.82	-7.14		-13.63
p-cresol	Cc1ccc(O)cc1	iodobenzene	-7.07	-7.17		-13.67
2-furaldehyde	O=Cc1occc1	iodobenzene	-6.17	-5.38		-10.36
5-methylfurfural	Cc1oc(C=O)cc1	iodobenzene	-6.98	-6.71		-12.39
helium	[He]	hexafluorobenzene	1.84	1.22		0.74
argon	[Ar]	hexafluorobenzene	0.40	0.80		0.39
krypton	[Kr]	hexafluorobenzene	-0.13	0.29		-0.19
oxygen	O=O	hexafluorobenzene	0.40	-0.23		-2.70
nitrogen	N#N	hexafluorobenzene	0.56	2.25		3.28
carbon monoxide	[C-]#[O+]	hexafluorobenzene	0.48	-0.18		-1.82
carbon dioxide	O=C=O	hexafluorobenzene	-0.93	-1.39		-4.55
methane	C	hexafluorobenzene	0.12	0.30		-0.22
perfluoroethane	FC(F)(F)C(F)(F)F	hexafluorobenzene	-0.71	1.32		1.60
octane	CCCCCCCC	hexafluorobenzene	-4.83	-4.30		-6.90
methyl ethyl ketone	CCC(C)=O	hexafluorobenzene	-4.33	-3.34		-6.19
toluene	Cc1ccccc1	hexafluorobenzene	-5.34	-4.23		-7.07
1,4-dioxane	C1COCCO1	hexafluorobenzene	-4.92	-4.30		-7.65
nitromethane	C[N+](=O)[O-]	hexafluorobenzene	-4.14	-3.14		-6.80
helium	[He]	chloroform	2.10	1.94		1.86
argon	[Ar]	chloroform	0.83	0.58		-0.19
krypton	[Kr]	chloroform	-0.01	-0.03		-1.11
xenon	[Xe]	chloroform	-0.72	-1.08		-2.74
radon	[Rn]	chloroform	-1.53	-1.25		-2.94
hydrogen	[H][H]	chloroform	1.61	1.51		1.09
oxygen	O=O	chloroform	0.96	0.78		0.02
nitrous oxide	[O-][N+]#N	chloroform	-0.97	-0.70		-1.79
carbon monoxide	[C-]#[O+]	chloroform	0.97	0.46		-0.45
carbon dioxide	O=C=O	chloroform	-0.61	-0.77		-2.72
hexane	CCCCCC	chloroform	-3.92	-3.70	-6.75	-6.97
2-methylpentane	CCCC(C)C	chloroform	-3.70	-3.53		-6.69
heptane	CCCCCCC	chloroform	-4.62	-4.40	-7.88	-8.10
2,4-dimethylpentane	CC(C)CC(C)C	chloroform	-4.15	-4.02		-7.48
octane	CCCCCCCC	chloroform	-5.32	-5.04	-8.98	-9.18
2,3,4-trimethylpentane	CC(C)C(C)(C)C	chloroform	-4.95	-4.44		-8.16
nonane	CCCCCCCCC	chloroform	-6.03	-5.77	-10.03	-10.30
cyclohexane	C1CCCCC1	chloroform	-4.45	-4.29	-7.24	-7.74
ethylcyclohexane	CCC1CCCCC1	chloroform	-5.44	-5.50		-9.66
dichloromethane	ClCCl	chloroform	-3.67	-3.27	-7.25	-6.11
trichloromethane	ClC(Cl)Cl	chloroform	-4.19	-4.05		-7.34
tetrachloromethane	ClC(Cl)(Cl)Cl	chloroform	-4.43	-4.40		-7.99
1,2-dichloroethane	ClCCCl	chloroform	-4.69	-4.41	-8.52	-7.90
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	chloroform	-4.42	-5.31		-9.31
1,1,2-trichloroethane	ClCC(Cl)Cl	chloroform	-5.28	-5.40		-9.35
1-chloropropane	CCCCl	chloroform	-3.62	-3.72		-7.08
bromoethane	CCBr	chloroform	-3.77	-3.40	-6.67	-6.65
iodomethane	CI	chloroform	-3.79	-3.49		-6.28
diethyl ether	CCOCC	chloroform	-4.16	-3.91	-8.70	-7.38
diisopropyl ether	CC(C)OC(C)C	chloroform	-4.94	-4.80	-9.87	-8.89
methyl <i>tert</i> -butyl ether	COC(C)(C)C	chloroform	-4.88	-3.97	-9.21	-7.54
tetrahydrofuran	C1CCOC1	chloroform	-5.27	-4.70	-10.18	-8.60
tetrahydropyran	C1CCOCC1	chloroform	-5.84	-5.32	-10.51	-9.58
1,4-dioxane	C1COCCO1	chloroform	-6.06	-5.37	-11.88	-9.64
butanone	CCC(C)=O	chloroform	-5.28	-4.67		-8.49
propylene carbonate	CC1COC(=O)O1	chloroform	-7.58	-7.16		-12.94
δ-pentanolactone	CC1CCC(=O)O1	chloroform	-8.73	-6.88		-12.20
methyl acetate	COC(C)=O	chloroform	-4.72	-4.46	-9.48	-8.16
ethyl acetate	CCOC(C)=O	chloroform	-5.43	-4.99	-10.48	-9.06
propyl acetate	CCCOC(C)=O	chloroform	-6.29	-5.63	-11.80	-10.16
butyl acetate	CCCCOC(C)=O	chloroform	-6.81	-6.23		-11.15
pentyl acetate	CCCCCOC(C)=O	chloroform	-7.42	-6.85		-12.17
methyl pentanoate	CCCCC(OC)=O	chloroform	-6.67	-6.28	-12.57	-11.16
methyl hexanoate	CCCCCC(=O)OC	chloroform	-7.24	-6.95	-13.85	-12.23
ethyl acetoacetate	CCOC(=O)CC(C)=O	chloroform	-7.90	-7.52		-13.15
ethyl trifluoroacetate	CCOC(=O)C(F)(F)F	chloroform	-4.15	-4.34		-11.40
ethyl trichloroacetate	CCOC(=O)C(Cl)(Cl)Cl	chloroform	-7.13	-7.68		-13.08
acetonitrile	CC#N	chloroform	-4.43	-4.51	-8.83	-7.50
ammonia	N	chloroform	-2.41	-2.27		-4.60
methylamine	CN	chloroform	-3.16	-2.83		-5.70
ethylamine	CCN	chloroform	-4.02	-3.42		-6.87
dimethylamine	CNC	chloroform	-3.70	-3.47		-7.19
diethylamine	CCNCC	chloroform	-5.16	-4.46		-9.17
diisopropylamine	CC(C)NC(C)C	chloroform	-5.42	-4.75		-10.10
trimethylamine	CN(C)C	chloroform	-3.90	-3.46		-7.12
acetamide	CC(N)=O	chloroform	-7.60	-7.18		-13.80
propionamide	CCC(N)=O	chloroform	-7.48	-7.82		-14.93

<i>N,N</i> -dimethylacetamide	CN(C)C(C)=O	chloroform	-8.06	-6.85		-13.03
2,2,2-trichloroacetamide	NC(=O)C(Cl)(Cl)Cl	chloroform	-6.92	-8.66		-14.88
ethyl carbamate	CCOC(N)=O	chloroform	-7.73	-8.46		-15.97
formic acid	OC=O	chloroform	-4.38	-3.64		-7.15
acetic acid	CC(O)=O	chloroform	-4.71	-4.68		-9.07
butanoic acid	CCCC(O)=O	chloroform	-5.99	-5.99		-11.43
2-methylpropanoic acid	CC(C)C(O)=O	chloroform	-5.80	-5.87		-11.32
pentanoic acid	CCCCC(O)=O	chloroform	-6.60	-6.58		-12.45
3-methylbutanoic acid	CC(C)CC(O)=O	chloroform	-6.36	-6.34		-12.25
hexanoic acid	CCCCC(O)=O	chloroform	-7.61	-7.17		-13.58
2-methylpentanoic acid	CCCC(C)C(O)=O	chloroform	-6.98	-6.99		-13.29
octanoic acid	CCCCCCCC(O)=O	chloroform	-9.02	-8.61		-15.77
chloroacetic acid	OC(=O)CCl	chloroform	-6.70	-5.27		-9.55
water	O	chloroform	-2.10	-3.00		-7.15
methanol	CO	chloroform	-3.29	-2.69	-6.86	-5.79
methanol	CO	chloroform	-3.42	-2.69	-6.86	-5.79
ethanol	CCO	chloroform	-3.82	-3.48	-7.84	-7.20
ethanol	CCO	chloroform	-4.01	-3.48	-7.84	-7.20
1-propanol	CCCO	chloroform	-4.45	-4.27	-8.41	-8.52
isopropanol	CC(C)O	chloroform	-4.27	-3.97	-8.39	-8.06
1-butanol	CCCCO	chloroform	-5.29	-4.93	-10.04	-9.64
isobutanol	CC(C)CO	chloroform	-4.97	-4.84		-9.46
2-butanol	CCC(C)O	chloroform	-5.03	-4.68		-9.20
2-methyl-isopropanol	CC(C)(C)O	chloroform	-4.45	-4.41		-8.98
1-hexanol	CCCCCCO	chloroform	-6.71	-6.31	-12.05	-11.76
1-heptanol	CCCCCCCO	chloroform	-7.50	-6.90		-12.79
3-methyl-1-pentanol	CCC(C)CCO	chloroform	-6.61	-5.97		-11.25
2-methyl-2-pentanol	CCCC(C)(C)O	chloroform	-5.69	-5.59		-10.96
3-methyl-2-pentanol	CCC(C)(C)CO	chloroform	-6.50	-5.53		-10.65
4-methyl-1-pentanol	CC(C)CCCO	chloroform	-6.60	-6.03		-11.30
2-methyl-3-pentanol	CCC(O)C(C)C	chloroform	-6.33	-5.55		-10.75
2,3-dimethyl-2-butanol	CC(C)(C)(C)CO	chloroform	-6.10	-5.26		-10.41
3,3-dimethyl-1-butanol	CC(C)(C)CCO	chloroform	-6.54	-5.84		-11.56
3-methyl-3-hexanol	CCCC(C)(O)CC	chloroform	-6.84	-6.16		-11.94
2-methyl-3-hexanol	CCCC(O)C(C)C	chloroform	-7.03	-6.21		-11.84
3-methyl-2-hexanol	CCCC(C)C(C)O	chloroform	-7.10	-6.25		-11.90
2-methyl-2-hexanol	CCCCC(C)(C)O	chloroform	-6.69	-6.05		-11.84
4,4-dimethyl-2-pentanol	CC(O)CC(C)(C)C	chloroform	-7.06	-6.05		-11.97
2,3-dimethyl-3-pentanol	CCC(C)(O)C(C)C	chloroform	-6.86	-5.71		-11.15
2,2-dimethyl-3-pentanol	CCC(O)C(C)(C)C	chloroform	-6.65	-6.08		-11.98
2-propen-1-ol	OCC=C	chloroform	-4.34	-4.23		-8.12
3-chloro-1-propanol	OCCCCl	chloroform	-5.84	-5.86		-10.84
1,3-propanediol	OCCCO	chloroform	-7.00	-6.71		-13.86
tributylphosphine oxide	CCCC[P](=O)(CCCC)CCCC	chloroform	-15.29	-8.99		-15.04
triethyl phosphate	CCO[P](=O)(OCC)OCC	chloroform	-10.65	-8.76		-13.11
benzene	c1ccccc1	chloroform	-4.79	-4.57	-8.57	-8.28
toluene	Cc1ccccc1	chloroform	-5.54	-5.17	-9.82	-9.19
ethylbenzene	CCc1ccccc1	chloroform	-5.84	-5.81		-10.14
1,3-dimethylbenzene	Cc1cccc(C)c1	chloroform	-5.85	-5.78		-10.12
fluorobenzene	Fc1ccccc1	chloroform	-4.69	-5.06		-9.20
chlorobenzene	Clc1ccccc1	chloroform	-5.76	-5.71		-9.92
1,3-dichlorobenzene	Clc1cccc(Cl)c1	chloroform	-6.26	-6.95		-11.78
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	chloroform	-6.32	-6.97		-11.81
2-chloronaphthalene	Clc1ccc2ccccc2c1	chloroform	-9.03	-9.07		-15.26
bromobenzene	Brc1ccccc1	chloroform	-6.41	-6.22		-10.85
iodobenzene	Ic1ccccc1	chloroform	-6.62	-7.16		-11.83
anisole	COc1ccccc1	chloroform	-6.71	-6.46	-12.06	-11.14
ethyl phenyl ether	CCOc1ccccc1	chloroform	-7.16	-7.09		-12.15
benzaldehyde	O=Cc1ccccc1	chloroform	-7.09	-7.13		-12.12
2-methoxybenzaldehyde	COc1ccccc1C=O	chloroform	-9.45	-8.62		-14.52
acetophenone	CC(=O)c1ccccc1	chloroform	-8.39	-7.90		-13.37
methyl benzoate	COC(=O)c1ccccc1	chloroform	-7.75	-8.15	-14.77	-13.79
phenyl acetate	CC(=O)Oc1ccccc1	chloroform	-8.51	-8.04		-13.58
dimethyl phthalate	COC(=O)c1ccccc1C(=O)OC	chloroform	-11.84	-10.67		-17.97
diethyl phthalate	CCOC(=O)c1ccccc1C(=O)OCC	chloroform	-12.82	-11.39		-19.46
benzonitrile	N#Cc1ccccc1	chloroform	-7.84	-8.23		-13.16
1,2-dicyanobenzene	N#Cc1ccccc1C#N	chloroform	-11.19	-9.94		-15.06
1,3-dicyanobenzene	N#Cc1cccc(c1)C#N	chloroform	-10.42	-10.11		-15.03
1,4-dicyanobenzene	N#Cc1ccc(cc1)C#N	chloroform	-11.32	-10.07		-14.90
2-methylaniline	Cc1ccccc1N	chloroform	-8.21	-7.47		-13.06
4-methylaniline	Cc1ccc(N)cc1	chloroform	-8.24	-7.67		-13.09
4-ethylaniline	CCc1ccc(N)cc1	chloroform	-8.57	-8.27		-14.07
4-propylaniline	CCCc1ccc(N)cc1	chloroform	-9.51	-8.88		-15.04
4-isopropylaniline	CC(C)c1ccc(N)cc1	chloroform	-9.15	-8.80		-14.98
4-butylaniline	CCCCc1ccc(N)cc1	chloroform	-9.85	-9.51		-16.05
4-chloroaniline	Nc1ccc(Cl)cc1	chloroform	-8.76	-8.44		-14.19
2-nitroaniline	Nc1ccccc1[N+](=O)[O-]	chloroform	-9.88	-10.25		-18.07
3-nitroaniline	Nc1cccc(c1)[N+](=O)[O-]	chloroform	-11.04	-10.47		-18.62
4-nitroaniline	Nc1ccc(cc1)[N+](=O)[O-]	chloroform	-12.00	-10.46		-18.53
3-aminoacetophenone	CC(=O)c1cccc(N)c1	chloroform	-11.09	-10.76		-18.51
<i>n</i> -methylaniline	CNc1ccccc1	chloroform	-7.97	-7.59	-13.57	-13.48
<i>N,N</i> -dimethylaniline	CN(C)c1ccccc1	chloroform	-8.20	-7.60	-13.92	-13.50
<i>N,N</i> -diethylaniline	CCN(CC)c1ccccc1	chloroform	-9.06	-8.69		-15.57

benzylamine	<chem>NCc1ccccc1</chem>	chloroform	-7.95	-7.55		-13.23
nitrobenzene	<chem>[O-][N+](=O)c1ccccc1</chem>	chloroform	-7.79	-7.50	-14.15	-12.88
3-nitrotoluene	<chem>Cc1ccc(c1)[N+](=[O-])=O</chem>	chloroform	-8.16	-8.37		-14.29
4-nitrotoluene	<chem>Cc1ccc(cc1)[N+](=[O-])=O</chem>	chloroform	-8.40	-8.33		-14.22
4-methylphenol	<chem>Cc1ccc(O)cc1</chem>	chloroform	-7.58	-7.30		-12.78
2,4-dimethylphenol	<chem>Cc1ccc(O)c(C)c1</chem>	chloroform	-8.06	-7.75		-13.55
2,5-dimethylphenol	<chem>Cc1ccc(C)c(O)c1</chem>	chloroform	-8.09	-7.85		-13.73
3-ethylphenol	<chem>CCc1ccc(O)c1</chem>	chloroform	-8.19	-7.98		-13.89
4-ethylphenol	<chem>CCc1ccc(O)cc1</chem>	chloroform	-8.14	-8.02		-13.92
3-chlorophenol	<chem>Oc1cccc(Cl)c1</chem>	chloroform	-8.01	-7.68		-13.20
2-bromophenol	<chem>Oc1ccccc1Br</chem>	chloroform	-7.33	-8.81		-15.39
2-iodophenol	<chem>Oc1ccccc1I</chem>	chloroform	-8.89	-9.89		-16.72
2,4-dichlorophenol	<chem>Oc1ccc(Cl)cc1Cl</chem>	chloroform	-7.83	-8.79		-14.63
2-methoxyphenol	<chem>COc1ccccc1O</chem>	chloroform	-7.90	-8.54	-14.81	-15.61
3-methoxyphenol	<chem>COc1ccc(O)c1</chem>	chloroform	-8.72	-8.90		-15.90
4-methoxyphenol	<chem>COc1ccc(O)cc1</chem>	chloroform	-9.02	-9.00		-16.02
2-hydroxybenzaldehyde	<chem>Oc1ccc(C=O)cc1</chem>	chloroform	-7.76	-8.19		-14.40
4-hydroxyacetophenone	<chem>CC(=O)c1ccc(O)cc1</chem>	chloroform	-11.05	-9.93		-17.16
2-nitrophenol	<chem>Oc1ccccc1[N+](=[O-])=O</chem>	chloroform	-8.03	-7.96		-13.86
4-nitrophenol	<chem>Oc1ccc(cc1)[N+](=[O-])=O</chem>	chloroform	-10.93	-9.28		-16.28
2,4-dinitrophenol	<chem>Oc1ccc(cc1[N+](=[O-])=O)[N+](=[O-])=O</chem>	chloroform	-10.68	-10.58		-18.65
2-hydroxybenzoic acid	<chem>OC(=O)c1ccccc1O</chem>	chloroform	-8.14	-8.86		-16.32
resorcinol	<chem>Oc1ccc(O)c1</chem>	chloroform	-9.56	-9.20		-17.02
benzyl alcohol	<chem>OCc1ccccc1</chem>	chloroform	-7.94	-7.57		-13.38
2-hydroxybenzyl alcohol	<chem>OCc1ccccc1O</chem>	chloroform	-9.49	-9.36		-18.06
2-methylpyridine	<chem>Cc1cccn1</chem>	chloroform	-6.90	-6.84	-12.67	-11.64
3-methylpyridine	<chem>Cc1ccncc1</chem>	chloroform	-7.35	-6.82	-13.21	-11.55
4-methylpyridine	<chem>Cc1ccncc1</chem>	chloroform	-7.50	-6.82	-13.36	-11.54
2-chloropyridine	<chem>Clc1cccn1</chem>	chloroform	-7.12	-7.25		-12.11
2-bromopyridine	<chem>BrC1=CC=CC=N1</chem>	chloroform	-7.99	-7.88		-13.13
2-methoxypyridine	<chem>COc1cccn1</chem>	chloroform	-6.74	-9.20		-16.04
piperidine	<chem>C1CCNCC1</chem>	chloroform	-6.37	-6.20	-11.83	-11.60
n-methyl-2-pyridone	<chem>CN1C=CC=CC1=O</chem>	chloroform	-9.36	-8.55		-15.13
quinoline	<chem>c1ccc2ncccc2c1</chem>	chloroform	-9.52	-9.75		-16.21
isoquinoline	<chem>c1ccc2cncccc2c1</chem>	chloroform	-9.41	-9.58		-15.88
pyrrole	<chem>[nH]1ccccc1</chem>	chloroform	-5.62	-5.90	-9.83	-10.44
trichlorofluoromethane	<chem>FC(Cl)(Cl)Cl</chem>	chloroform	-2.82	-3.14		-6.33
dichlorodifluoromethane	<chem>FC(F)(Cl)Cl</chem>	chloroform	-1.71	-1.69		-4.22
hcn	<chem>C#N</chem>	chloroform	-3.14	-3.14		-5.23
helium	<chem>[He]</chem>	dichloromethane	2.04	1.94	2.68	1.85
hydrogen	<chem>[H][H]</chem>	dichloromethane	1.56	1.48	2.12	1.08
nitrogen	<chem>N#N</chem>	dichloromethane	1.21	0.87	1.41	0.64
oxygen	<chem>O=O</chem>	dichloromethane	0.90	0.85	0.85	0.25
carbon dioxide	<chem>O=C=O</chem>	dichloromethane	-0.68	-1.04	-2.62	-3.08
pentane	<chem>CCCCC</chem>	dichloromethane	-3.06	-2.83	-4.79	-5.44
hexane	<chem>CCCCCC</chem>	dichloromethane	-3.74	-3.53	-5.86	-6.55
heptane	<chem>CCCCCCC</chem>	dichloromethane	-4.46	-4.22	-6.83	-7.67
2,4-dimethylpentane	<chem>CC(C)CC(C)C</chem>	dichloromethane	-3.98	-3.80		-6.98
octane	<chem>CCCCCCCC</chem>	dichloromethane	-5.07	-4.85	-7.81	-8.73
2,5-dimethylhexane	<chem>CC(C)CCC(C)C</chem>	dichloromethane	-4.64	-4.50		-8.10
2,3,4-trimethylpentane	<chem>CC(C)C(C)C(C)C</chem>	dichloromethane	-4.74	-4.17		-7.61
nonane	<chem>CCCCCCCCC</chem>	dichloromethane	-5.75	-5.57	-8.85	-9.85
ethylcyclohexane	<chem>CCC1CCCCC1</chem>	dichloromethane	-5.22	-5.36		-9.30
benzene	<chem>c1ccccc1</chem>	dichloromethane	-4.80	-4.58	-7.96	-8.11
chlorobenzene	<chem>Clc1ccccc1</chem>	dichloromethane	-5.90	-5.83	-9.52	-9.96
diethyl ether	<chem>CCOCC</chem>	dichloromethane	-3.91	-4.07	-7.09	-7.50
dipropyl ether	<chem>CCCOCC</chem>	dichloromethane	-5.03	-5.29		-9.52
methyl butyl ether	<chem>CCCCOC</chem>	dichloromethane	-4.71	-4.71		-8.56
diethoxymethane	<chem>CCOCCOC</chem>	dichloromethane	-5.47	-5.37		-9.46
1,2-dimethoxyethane	<chem>COCOCOC</chem>	dichloromethane	-5.82	-5.35		-9.42
dichloromethane	<chem>ClCCl</chem>	dichloromethane	-3.86	-3.38	-6.88	-6.13
methanol	<chem>CO</chem>	dichloromethane	-3.12	-3.12	-6.17	-6.48
ethanol	<chem>CCO</chem>	dichloromethane	-3.71	-3.84	-7.07	-7.78
2-ethoxyethanol	<chem>CCOCCO</chem>	dichloromethane	-6.06	-6.56		-12.60
toluene	<chem>Cc1ccccc1</chem>	dichloromethane	-5.49	-5.20	-9.20	-9.08
nitromethane	<chem>C[N+](=[O-])=O</chem>	dichloromethane	-4.93	-5.00	-8.95	-9.21
2-butanol	<chem>CCC(C)O</chem>	1-chlorobutane	-4.17	-4.84		-9.63
isobutanol	<chem>CC(C)CO</chem>	1-chlorobutane	-4.41	-5.03		-9.92
1-butanol	<chem>CCCCO</chem>	1-chlorobutane	-4.60	-5.13		-10.12
methyl iodide	<chem>CI</chem>	1-chlorobutane	-3.44	-3.35		-5.98
nitromethane	<chem>C[N+](=[O-])=O</chem>	1-chlorobutane	-4.06	-4.56		-8.49
ethyl iodide	<chem>CCI</chem>	1-chlorobutane	-4.10	-3.91		-6.79
acetone	<chem>CC(C)=O</chem>	1-chlorobutane	-3.62	-3.80		-6.93
1-chloropropane	<chem>CCCCl</chem>	1-chlorobutane	-3.69	-3.66		-6.96
cyclohexane	<chem>C1CCCCC1</chem>	1-chlorobutane	-4.18	-4.01		-7.26
hexane	<chem>CCCCCC</chem>	1-chlorobutane	-3.86	-3.35		-6.37
triethylamine	<chem>CCN(CC)CC</chem>	1-chlorobutane	-4.57	-4.88		-9.86
cyclohexene	<chem>C1CCC=CC1</chem>	1-chlorobutane	-4.37	-4.11		-7.34
benzene	<chem>c1ccccc1</chem>	1-chlorobutane	-4.46	-4.38		-7.86
1-chlorobutane	<chem>CCCCl</chem>	1-chlorobutane	-4.42	-4.32		-8.02
aniline	<chem>Nc1ccccc1</chem>	1-chlorobutane	-6.67	-6.96		-11.67
ethyl acetate	<chem>CCOC(C)=O</chem>	1-chlorobutane	-4.33	-4.76		-8.40

toluene	Cc1ccccc1	1-chlorobutane	-5.15	-4.86		-8.52
acetonitrile	CC#N	1-chlorobutane	-3.63	-4.35		-6.89
pentane	CCCCC	1-chlorobutane	-3.21	-2.65		-5.26
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	1-chlorobutane	-4.58	-4.22		-8.12
2,2,4-trimethyl-2-pentene	CC(C)(C)/C=C(C)/C	1-chlorobutane	-4.75	-4.54		-8.54
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	1-chlorobutane	-4.33	-5.13		-8.88
1-hexanol	CCCCCCO	1-chlorobutane	-5.98	-6.48		-12.20
ethanol	CCO	1-chlorobutane	-3.07	-3.71		-7.72
1-octanol	CCCCCCCCO	1-chlorobutane	-7.22	-7.70		-14.19
diethyl ether	CCOCC	1-chlorobutane	-3.39	-3.84		-7.20
diisopropyl ether	CC(C)OC(C)C	1-chlorobutane	-4.12	-4.35		-8.02
diethoxymethane	CCOCCOC	1-chlorobutane	-4.67	-5.04		-8.91
1,2-dimethoxyethane	COCCOC	1-chlorobutane	-4.61	-4.92		-8.67
1,4-dioxane	C1COCCO1	1-chlorobutane	-4.80	-5.07		-8.91
2-chlorobutane	CCC(C)Cl	1-chlorobutane	-4.16	-4.21		-7.85
cyclopentanone	O=C1CCCC1	1-chlorobutane	-5.46	-5.91		-10.23
1,2-dichloroethane	ClCCCl	1-chlorobutane	-4.42	-4.43		-7.89
iodine	I2	1-chlorobutane	-5.64	-5.43		-8.98
hexachlorobenzene	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	1-chlorobutane	-10.63	-9.27		-15.59
diuron	CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1	1-chlorobutane	-13.31	-13.67		-24.41
carbon tetrachloride	ClC(Cl)(Cl)Cl	1-chlorobutane	-4.29	-4.01		-7.25
helium	[He]	carbon tetrachloride	2.13	1.94		1.86
argon	[Ar]	carbon tetrachloride	0.64	0.58	-0.10	-0.20
krypton	[Kr]	carbon tetrachloride	-0.16	-0.03		-1.11
xenon	[Xe]	carbon tetrachloride	-0.71	-1.04		-2.69
hydrogen	[H][H]	carbon tetrachloride	1.51	1.51	1.38	1.08
oxygen	O=O	carbon tetrachloride	0.71	0.77	0.01	-0.03
nitrous oxide	[O-][N+][N]	carbon tetrachloride	-0.86	-0.58		-1.77
nitric oxide	[N]=O	carbon tetrachloride	0.61	0.33	-0.34	-0.64
carbon monoxide	[C-]#[O+]	carbon tetrachloride	0.90	0.62	0.30	-0.23
carbon dioxide	O=C=O	carbon tetrachloride	-0.61	-0.27	-2.25	-1.81
iodine	I2	carbon tetrachloride	-5.26	-5.56		-9.20
methane	C	carbon tetrachloride	0.19	0.22	-0.72	-0.79
tetrafluoromethane	FC(F)(F)F	carbon tetrachloride	0.82	0.91		-0.12
sulfur hexafluoride	F[S](F)(F)(F)(F)F	carbon tetrachloride	-0.03	-0.09	-1.67	-1.80
ethane	CC	carbon tetrachloride	-1.00	-0.73	-2.20	-2.30
propane	CCC	carbon tetrachloride	-1.83	-1.54	-3.44	-3.58
butane	CCCC	carbon tetrachloride	-2.67	-2.32	-4.42	-4.82
2-methylpropane	CC(C)C	carbon tetrachloride	-2.37	-2.22		-4.66
2-methylpentane	CCCC(C)C	carbon tetrachloride	-3.83	-3.70		-6.99
2,4-dimethylpentane	CC(C)CC(C)C	carbon tetrachloride	-4.27	-4.27		-7.88
2,5-dimethylhexane	CC(C)CCC(C)C	carbon tetrachloride	-4.99	-5.00		-9.03
hexadecane	CCCCCCCCCCCCCCCC	carbon tetrachloride	-11.40	-10.90	-18.24	-18.43
cyclopentane	C1CCCC1	carbon tetrachloride	-3.76	-3.55	-6.80	-6.63
cyclohexane	C1CCCCC1	carbon tetrachloride	-4.39	-4.26	-7.73	-7.72
cyclodecane	C1CCCCCCCCC1	carbon tetrachloride	-7.42	-6.93	-12.43	-11.98
ethene	C=C	carbon tetrachloride	-0.78	-0.73	-2.29	-2.28
propene	CC=C	carbon tetrachloride	-1.84	-1.55		-3.58
1-butene	CCC=C	carbon tetrachloride	-2.50	-2.33		-4.82
2-methyl-1,3-butadiene	CC(=C)C=C	carbon tetrachloride	-3.49	-3.03		-5.94
acetylene	C#C	carbon tetrachloride	-0.65	-0.82		-2.47
chloromethane	CCl	carbon tetrachloride	-2.20	-1.67		-3.75
chloropropane	CCCCl	carbon tetrachloride	-3.70	-3.34		-6.45
2-chloro-2-methylpropane	CC(C)(C)Cl	carbon tetrachloride	-3.66	-3.73		-7.02
dichloromethane	ClCCl	carbon tetrachloride	-3.36	-2.93		-5.64
trichloromethane	ClC(Cl)Cl	carbon tetrachloride	-4.01	-3.71		-6.81
carbon tetrachloride	ClC(Cl)(Cl)Cl	carbon tetrachloride	-4.42	-4.33		-7.85
1,1-dichloroethane	CC(Cl)Cl	carbon tetrachloride	-3.78	-3.73		-6.83
1,2-dichloroethane	ClCCCl	carbon tetrachloride	-4.30	-3.94		-7.20
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	carbon tetrachloride	-4.24	-4.87		-8.67
1,1,2-trichloroethane	ClCC(Cl)Cl	carbon tetrachloride	-5.06	-4.89		-8.57
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	carbon tetrachloride	-5.93	-5.87		-10.04
1,3-dichloropropane	ClCCCCl	carbon tetrachloride	-5.20	-4.68		-8.38
1-chlorobutane	CCCCCl	carbon tetrachloride	-4.31	-4.09	-7.93	-7.62
dibromomethane	BrCBr	carbon tetrachloride	-4.69	-4.66		-8.83
1-bromopropane	CCCBBr	carbon tetrachloride	-4.17	-3.97		-7.59
2-bromo-2-methylpropane	CC(C)(C)Br	carbon tetrachloride	-4.13	-4.13		-7.70
1-bromobutane	CCCCBr	carbon tetrachloride	-4.75	-4.56		-8.47
1,2-dibromoethane	BrCCBr	carbon tetrachloride	-5.34	-5.50		-9.95
iodomethane	CI	carbon tetrachloride	-3.45	-3.42	-6.48	-6.24
1-iodopropane	CCCI	carbon tetrachloride	-4.97	-4.71		-8.19
1-iodobutane	CCCCI	carbon tetrachloride	-5.57	-5.46	-9.65	-9.36
trifluorochloromethane	FC(F)(F)Cl	carbon tetrachloride	-0.60	-0.35		-2.26
difluorodichloromethane	FC(F)(Cl)Cl	carbon tetrachloride	-1.92	-1.74		-4.29
1,1,2-trifluoro-1,2-dichloroethane	FC(F)(Cl)C(F)(Cl)Cl	carbon tetrachloride	-3.27	-3.36		-6.81
bromochloromethane	ClCBr	carbon tetrachloride	-3.92	-3.87		-7.44
diethyl ether	CCOCC	carbon tetrachloride	-3.52	-3.56	-6.92	-6.86
dipropyl ether	CCCOCCC	carbon tetrachloride	-4.83	-4.89	-8.77	-8.93
diisopropyl ether	CC(C)OC(C)C	carbon tetrachloride	-4.23	-4.46		-8.23
dibutyl ether	CCCCOCCCC	carbon tetrachloride	-6.28	-6.20	-11.10	-10.98
methyl butyl ether	CCCCOC	carbon tetrachloride	-4.39	-4.28		-8.00
ethyl butyl ether	CCCCOCC	carbon tetrachloride	-4.91	-4.78		-8.76
dimethoxymethane	COCOC	carbon tetrachloride	-3.66	-3.45	-7.27	-6.64

diethoxymethane	CCOCCOC	carbon tetrachloride	-4.97	-4.54		-8.25
1,2-dimethoxyethane	COCCOC	carbon tetrachloride	-4.64	-4.23	-8.96	-7.80
tetrahydrofuran	C1CCOC1	carbon tetrachloride	-4.27	-4.28	-8.27	-8.05
1,4-dioxane	C1COCCO1	carbon tetrachloride	-4.97	-4.77	-9.06	-8.82
methyl <i>tert</i> -butyl ether	COC(C)(C)C	carbon tetrachloride	-3.95	-3.68	-6.88	-7.01
propanone	CC(C)=O	carbon tetrachloride	-3.25	-3.13		-6.12
butanone	CCC(C)=O	carbon tetrachloride	-4.08	-3.99		-7.53
2-hexanone	CCCCC(C)=O	carbon tetrachloride	-5.36	-5.41	-10.00	-9.78
cyclopentanone	O=C1CCCC1	carbon tetrachloride	-5.54	-4.99	-9.89	-8.90
cyclohexanone	O=C1CCCCC1	carbon tetrachloride	-6.23	-5.72	-10.68	-10.05
acetonitrile	CC#N	carbon tetrachloride	-3.03	-3.17	-6.06	-5.50
propionitrile	CCC#N	carbon tetrachloride	-3.78	-3.80		-6.46
dimethylamine	CNC	carbon tetrachloride	-2.88	-2.76		-5.89
trimethylamine	CN(C)C	carbon tetrachloride	-2.89	-3.06		-6.35
triethylamine	CCN(CC)CC	carbon tetrachloride	-4.83	-4.72	-9.09	-9.11
nitromethane	C[N+](=[O-])=O	carbon tetrachloride	-3.46	-3.16	-6.78	-6.38
2-nitropropane	CC(C)[N+](=[O-])=O	carbon tetrachloride	-4.57	-4.61	-8.57	-8.75
ethanol	CCO	carbon tetrachloride	-2.81	-2.58	-5.80	-5.52
1-propanol	CCCO	carbon tetrachloride	-3.53	-3.36	-6.67	-6.79
1-butanol	CCCCO	carbon tetrachloride	-4.45	-4.08	-8.25	-7.99
2-methyl-isopropanol	CC(C)(C)O	carbon tetrachloride	-3.52	-3.75		-7.65
1-hexanol	CCCCCCO	carbon tetrachloride	-5.74	-5.52	-10.09	-10.22
2-ethoxyethanol	CCOCCO	carbon tetrachloride	-4.87	-5.17		-10.09
toluene	Cc1ccccc1	carbon tetrachloride	-5.21	-4.94	-9.11	-8.96
1,4-dimethylbenzene	Cc1ccc(C)cc1	carbon tetrachloride	-5.73	-5.57		-9.92
naphthalene	c1ccc2ccccc2c1	carbon tetrachloride	-7.63	-7.41	-12.94	-12.92
biphenyl	c1ccc(cc1)c2ccccc2	carbon tetrachloride	-9.22	-8.83	-15.07	-15.04
phenanthrene	c1ccc2c(c1)ccc3ccccc23	carbon tetrachloride	-10.98	-10.48		-17.74
anthracene	c1ccc2cc3ccccc3cc2c1	carbon tetrachloride	-11.15	-10.46	-18.45	-17.69
1,2-dichlorobenzene	Clc1ccccc1Cl	carbon tetrachloride	-6.79	-6.35	-11.03	-11.03
bromobenzene	Brc1ccccc1	carbon tetrachloride	-6.23	-5.87	-10.27	-10.42
iodobenzene	Ic1ccccc1	carbon tetrachloride	-6.81	-6.68	-11.47	-11.12
ethyl formate	CCOC=O	carbon tetrachloride	-3.32	-3.63		-7.10
diethyl carbonate	CCOC(=O)OCC	carbon tetrachloride	-5.78	-5.24	-10.23	-9.73
dimethyl carbonate	COC(=O)OC	carbon tetrachloride	-4.25	-4.20		-8.07
mercury	[Hg]	carbon tetrachloride	-2.55	1.75		1.48
diethyl ether	CCOCC	carbon tetrachloride	-3.53	-3.56	-6.92	-6.86
pentanoic acid	CCCCC(O)=O	carbon tetrachloride	-5.59	-5.24		-9.92
phenol	Oc1ccccc1	carbon tetrachloride	-6.21	-5.56	-10.37	-10.00
2-chlorophenol	Oc1ccccc1Cl	carbon tetrachloride	-6.18	-6.24	-11.02	-10.82
3-chlorophenol	Oc1cccc(Cl)c1	carbon tetrachloride	-7.29	-6.52		-11.31
4-chlorophenol	Oc1ccc(Cl)cc1	carbon tetrachloride	-7.58	-6.54	-11.59	-11.34
1-nitropropane	CCC[N+](=[O-])=O	carbon tetrachloride	-4.69	-4.62	-9.14	-8.71
acetylacetone	CC(=O)CC(C)=O	carbon tetrachloride	-5.52	-5.93		-10.73
1,4-dioxane	C1COCCO1	carbon tetrachloride	-4.88	-4.77	-9.06	-8.82
benzyl alcohol	OCc1ccccc1	carbon tetrachloride	-6.59	-6.36		-11.31
methanol	CO	carbon tetrachloride	-2.24	-1.79	-4.73	-4.18
ethanol	CCO	carbon tetrachloride	-2.63	-2.58	-5.80	-5.52
1-propanol	CCCO	carbon tetrachloride	-3.60	-3.36	-6.67	-6.79
isopropanol	CC(C)O	carbon tetrachloride	-2.90	-3.18	-6.31	-6.54
1-butanol	CCCCO	carbon tetrachloride	-4.32	-4.08	-8.25	-7.99
2-methyl-isopropanol	CC(C)(C)O	carbon tetrachloride	-3.31	-3.75		-7.65
1-pentanol	CCCCCO	carbon tetrachloride	-5.11	-4.74	-9.04	-9.04
2-pentanol	CCCC(C)O	carbon tetrachloride	-4.71	-4.63		-8.88
1-hexanol	CCCCCCO	carbon tetrachloride	-5.83	-5.52	-10.09	-10.22
2-methyl-2-butanol	CCC(C)(C)O	carbon tetrachloride	-4.37	-4.35	-7.34	-8.64
2-methyl-2-pentanol	CCCC(C)(C)O	carbon tetrachloride	-5.16	-5.04		-9.75
4-methyl-1-pentanol	CC(C)CCCCO	carbon tetrachloride	-5.46	-5.35		-9.97
2-methyl-3-pentanol	CCC(O)C(C)C	carbon tetrachloride	-5.32	-5.01		-9.58
4-methyl-2-pentanol	CC(C)CC(C)O	carbon tetrachloride	-5.23	-5.15		-9.82
2,3-dimethyl-2-butanol	CC(C)(C)C(C)O	carbon tetrachloride	-5.16	-4.89		-9.54
3,3-dimethyl-1-butanol	CC(C)(C)CCO	carbon tetrachloride	-5.45	-5.18		-10.08
2-methyl-3-hexanol	CCCC(O)C(C)C	carbon tetrachloride	-6.43	-5.68		-10.65
2-methyl-2-hexanol	CCCCC(C)(C)O	carbon tetrachloride	-5.82	-5.62		-10.77
5-methyl-2-hexanol	CC(C)CCCCO	carbon tetrachloride	-6.07	-5.77		-10.75
3-ethyl-3-pentanol	CCC(O)(CC)CC	carbon tetrachloride	-6.02	-5.58		-10.68
4,4-dimethyl-2-pentanol	CC(O)CC(C)(C)C	carbon tetrachloride	-5.98	-5.46		-10.54
2,3-dimethyl-3-pentanol	CCC(C)(O)C(C)C	carbon tetrachloride	-5.96	-5.45		-10.47
2,2-dimethyl-3-pentanol	CCC(O)C(C)(C)C	carbon tetrachloride	-5.46	-5.55		-10.70
1-heptanol	CCCCCCCO	carbon tetrachloride	-6.36	-6.20		-11.37
1-octanol	CCCCCCCCO	carbon tetrachloride	-6.94	-6.89	-12.48	-12.43
formic acid	OC=O	carbon tetrachloride	-2.99	-2.28		-4.88
acetic acid	CC(O)=O	carbon tetrachloride	-3.06	-3.24		-6.54
propanoic acid	CCC(O)=O	carbon tetrachloride	-3.98	-3.97		-7.82
butanoic acid	CCCC(O)=O	carbon tetrachloride	-4.80	-4.57		-8.82
3-methylbutanoic acid	CC(C)CC(O)=O	carbon tetrachloride	-5.37	-5.10		-9.85
chlorine	ClCl	carbon tetrachloride	-1.90	-1.33		-3.21
acetophenone	CC(=O)c1ccccc1	carbon tetrachloride	-7.18	-6.99	-11.97	-12.16
acetone	CC(C)=O	carbon tetrachloride	-3.40	-3.13	-6.73	-6.12
2-pentanone	CCCC(C)=O	carbon tetrachloride	-4.80	-4.69	-8.86	-8.64
2-hexanone	CCCCC(C)=O	carbon tetrachloride	-5.47	-5.41	-10.00	-9.78
2-heptanone	CCCCCC(C)=O	carbon tetrachloride	-6.15	-6.06	-11.09	-10.79
germanium tetrabromide	Br[Ge](Br)(Br)Br	carbon tetrachloride	-7.11	-6.05		-11.38

chlorobenzene	Clc1ccccc1	carbon tetrachloride	-5.67	-5.35	-9.64	-9.50
1,3-dichlorobenzene	Clc1cccc(Cl)c1	carbon tetrachloride	-6.21	-6.50	-11.22	-11.22
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	carbon tetrachloride	-6.28	-6.52	-11.16	-11.24
bromobenzene	Brc1ccccc1	carbon tetrachloride	-6.34	-5.87	-10.27	-10.42
1,5-hexadiene	C=CCCC=C	carbon tetrachloride	-3.96	-3.92		-7.33
2-methylbut-2-ene	CC=C(C)C	carbon tetrachloride	-3.25	-3.08		-6.04
1-hexene	CCCCC=C	carbon tetrachloride	-3.82	-3.87		-7.25
methyl acetate	COC(C)=O	carbon tetrachloride	-3.63	-3.72	-7.39	-7.22
ethyl acetate	CCOC(C)=O	carbon tetrachloride	-4.24	-4.28	-8.36	-8.10
butyl acetate	CCCCOC(C)=O	carbon tetrachloride	-5.69	-5.55	-10.57	-10.10
pentyl acetate	CCCCCOC(C)=O	carbon tetrachloride	-6.40	-6.18		-11.09
methyl propanoate	CCC(=O)OC	carbon tetrachloride	-4.43	-4.32		-8.13
methyl pentanoate	CCCCC(=O)OC	carbon tetrachloride	-5.70	-5.59		-10.12
ammonia	N	carbon tetrachloride	-1.08	-1.06		-2.47
methylamine	CN	carbon tetrachloride	-2.52	-1.99		-4.28
ethylamine	CCN	carbon tetrachloride	-2.77	-2.66		-5.51
dimethylamine	CNC	carbon tetrachloride	-2.76	-2.76		-5.89
diethylamine	CCNCC	carbon tetrachloride	-4.12	-3.96	-7.94	-8.08
trimethylamine	CN(C)C	carbon tetrachloride	-3.07	-3.06		-6.35
triethylamine	CCN(CC)CC	carbon tetrachloride	-4.45	-4.72	-9.09	-9.11
4-methylphenol	Cc1ccc(O)cc1	carbon tetrachloride	-6.44	-6.23		-11.03
benzene	c1ccccc1	carbon tetrachloride	-4.49	-4.25	-7.96	-7.90
toluene	Cc1ccccc1	carbon tetrachloride	-5.29	-4.94	-9.11	-8.96
1,2-dimethylbenzene	Cc1ccccc1C	carbon tetrachloride	-6.18	-5.57		-9.94
pyridine	c1ccncc1	carbon tetrachloride	-5.14	-4.89	-9.16	-8.49
3-chloroaniline	Nc1cccc(Cl)c1	carbon tetrachloride	-7.69	-7.43		-12.69
4-chloroaniline	Nc1ccc(Cl)cc1	carbon tetrachloride	-7.69	-7.42		-12.70
2-methylaniline	Cc1ccccc1N	carbon tetrachloride	-7.15	-6.64		-11.75
4-methylaniline	Cc1ccc(N)cc1	carbon tetrachloride	-7.11	-6.81		-11.83
2-nitrotoluene	Cc1ccccc1[N+](=O)[O-]	carbon tetrachloride	-7.49	-7.39		-12.97
4-methylpyridine	Cc1cncnc1	carbon tetrachloride	-6.08	-5.69		-9.79
benzonitrile	N#Cc1ccccc1	carbon tetrachloride	-6.62	-6.66	-11.50	-10.90
benzamide	NC(=O)c1ccccc1	carbon tetrachloride	-9.24	-9.15		-16.11
benzaldehyde	O=Cc1ccccc1	carbon tetrachloride	-6.11	-6.12	-11.20	-10.70
nitrobenzene	[O-][N+](=O)c1ccccc1	carbon tetrachloride	-7.18	-6.34	-12.00	-11.20
methyl ethyl ketone	CCC(C)=O	carbon tetrachloride	-4.13	-3.99	-7.92	-7.52
methyl salicylate	COC(=O)c1ccccc1O	carbon tetrachloride	-7.38	-7.92		-14.21
ethyl salicylate	CCOC(=O)c1ccccc1O	carbon tetrachloride	-8.27	-8.46		-15.36
propyl salicylate	CCCOC(=O)c1ccccc1O	carbon tetrachloride	-8.96	-9.21		-16.30
butyl salicylate	CCCCOC(=O)c1ccccc1O	carbon tetrachloride	-9.73	-9.88		-17.96
methyl benzoate	COC(=O)c1ccccc1	carbon tetrachloride	-6.83	-7.25		-12.65
5-methylfurfural	Cc1oc(C=O)cc1	carbon tetrachloride	-6.40	-6.25		-11.12
2-furaldehyde	O=Cc1occc1	carbon tetrachloride	-5.54	-5.15		-9.48
trichloroacetic acid	OC(=O)C(Cl)(Cl)Cl	carbon tetrachloride	-6.53	-5.09		-9.04
water	O	carbon tetrachloride	-0.87	-1.52		-4.17
hydrogen peroxide	OO	carbon tetrachloride	-2.31	-0.92		-2.68
nitromethane	C[N+](=O)[O-]	carbon tetrachloride	-3.48	-3.16	-6.78	-6.38
n-methylaniline	CNc1ccccc1	carbon tetrachloride	-6.60	-6.55	-11.85	-11.71
2-aminophenol	Nc1ccccc1O	carbon tetrachloride	-7.82	-7.72		-13.97
4-aminophenol	Nc1ccc(O)cc1	carbon tetrachloride	-8.27	-8.03		-14.38
2-bromophenol	Oc1ccccc1Br	carbon tetrachloride	-7.09	-7.59		-13.34
4-nitrotoluene	Cc1ccc(cc1)[N+](=O)[O-]	carbon tetrachloride	-7.58	-7.15		-12.50
chloroacetic acid	OC(=O)CCl	carbon tetrachloride	-5.29	-3.95		-7.39
methyl ethyl ketone	CCC(C)=O	bromoethane	-4.67	-4.77		-8.54
toluene	Cc1ccccc1	bromoethane	-5.33	-4.98		-8.73
1,4-dioxane	C1COCCO1	bromoethane	-5.05	-5.34		-9.44
argon	[Ar]	methylene iodide	1.99	0.93		-0.68
methane	C	methylene iodide	1.46	0.73		-1.54
octane	CCCCCCCC	methylene iodide	-3.37	-4.52		-10.16
nonane	CCCCCCCCC	methylene iodide	-3.98	-5.38		-11.55
decane	CCCCCCCCC	methylene iodide	-4.60	-6.16		-12.81
undecane	CCCCCCCCCCC	methylene iodide	-5.21	-6.71		-13.73
dichloromethane	ClCCl	methylene iodide	-2.80	-2.64		-7.01
tetrachloromethane	ClC(Cl)(Cl)Cl	methylene iodide	-3.14	-3.64		-8.64
1,2-dichloroethane	ClCCCl	methylene iodide	-3.72	-4.17		-9.58
acetone	CC(C)=O	methylene iodide	-3.31	-3.68		-8.99
2-pentanone	CCCC(C)=O	methylene iodide	-4.22	-5.24		-11.49
methyl formate	COC=O	methylene iodide	-2.55	-2.93		-7.50
ethyl formate	CCOC=O	methylene iodide	-2.99	-3.48		-8.33
nitromethane	C[N+](=O)[O-]	methylene iodide	-3.79	-4.44		-10.55
nitroethane	CC[N+](=O)[O-]	methylene iodide	-4.28	-5.32		-11.97
methanol	CO	methylene iodide	-2.56	-2.09		-6.66
ethanol	CCO	methylene iodide	-2.91	-2.85		-7.98
1-propanol	CCCO	methylene iodide	-3.53	-3.60		-9.21
isopropanol	CC(C)O	methylene iodide	-2.96	-3.33		-8.83
2-butanol	CCC(C)O	methylene iodide	-3.63	-4.11		-10.13
1-pentanol	CCCCCO	methylene iodide	-4.77	-4.85		-11.20
2,2,2-trifluoroethanol	OCC(F)(F)F	methylene iodide	-2.54	-3.16		-9.83
1,1,1,3,3,3-hexafluoroisopropanol	OC(C(F)(F)F)C(F)(F)F	methylene iodide	-2.46	-2.76		-9.28
benzene	c1ccccc1	methylene iodide	-3.83	-3.83		-8.78
toluene	Cc1ccccc1	methylene iodide	-4.49	-4.65		-10.13
ethylbenzene	CCc1ccccc1	methylene iodide	-5.01	-5.40		-11.30



butylbenzene	CCCCc1ccccc1	methylene iodide	-5.88	-6.87		-13.63
3-chlorotoluene	Cc1cccc(Cl)c1	methylene iodide	-5.62	-6.28		-12.76
pentane	CCCCC	dibromomethane	-2.59	-2.72		-6.27
hexane	CCCCCC	dibromomethane	-3.30	-3.49		-7.52
heptane	CCCCCCC	dibromomethane	-3.94	-4.21		-8.70
cyclohexane	C1CCCCC1	dibromomethane	-4.04	-4.25		-8.60
carbon tetrachloride	ClC(Cl)(Cl)Cl	dibromomethane	-4.31	-3.99		-8.17
diethyl ether	CCOCC	dibromomethane	-3.44	-3.79		-8.03
dipropyl ether	CCCOCCC	dibromomethane	-4.56	-5.26		-10.51
dibutyl ether	CCCCOCCCC	dibromomethane	-5.81	-6.69		-12.89
tetrahydrofuran	C1CCOC1	dibromomethane	-4.73	-4.69		-9.45
3-pentanone	CCC(=O)CC	dibromomethane	-5.42	-5.54		-10.78
benzene	c1ccccc1	dibromomethane	-4.77	-4.37		-8.74
toluene	Cc1ccccc1	dibromomethane	-5.14	-5.18		-10.09
o-xylene	Cc1ccccc1C	dibromomethane	-6.82	-5.89		-11.25
dimethyl sulfoxide	C[S](C)=O	dibromomethane	-7.86	-7.66		-14.06
ethyl acetate	CCOC(C)=O	dibromomethane	-4.79	-4.81		-9.53
1-propanol	CCCO	dibromomethane	-4.24	-4.14		-9.16
1-butanol	CCCCO	dibromomethane	-4.83	-4.84		-10.36
bromochloromethane	ClCBr	dibromomethane	-4.38	-4.22		-8.86
dibromomethane	BrCBr	dibromomethane	-5.14	-5.03		-10.37
bromotrichloromethane	ClC(Cl)(Cl)Br	dibromomethane	-4.76	-4.77		-9.50
argon	[Ar]	diethyl ether	0.30	0.51		-0.17
radon	[Rn]	diethyl ether	-1.52	-1.44		-2.89
hydrogen	[H][H]	diethyl ether	1.15	1.04		0.52
carbon monoxide	[C-]#[O+]	diethyl ether	0.55	-0.08		-1.16
methane	C	diethyl ether	-0.03	-0.31		-1.76
ethane	CC	diethyl ether	-1.16	-1.19		-3.15
octane	CCCCCCCC	diethyl ether	-5.35	-5.36	-9.46	-9.62
cyclohexane	C1CCCCC1	diethyl ether	-4.19	-4.21	-7.48	-7.43
dichloromethane	ClCCl	diethyl ether	-3.87	-3.79		-7.36
tetrachloromethane	ClC(Cl)(Cl)Cl	diethyl ether	-4.39	-4.96	-8.21	-9.05
1-chlorobutane	CCCCCl	diethyl ether	-4.38	-4.37	-8.14	-8.20
2-chloro-2-methylpropane	CC(C)(C)Cl	diethyl ether	-3.38	-3.81		-7.26
2-bromo-2-methylpropane	CC(C)(C)Br	diethyl ether	-3.85	-4.27		-8.14
iodoethane	CCl	diethyl ether	-3.77	-3.86		-6.71
diethylether	CCOCC	diethyl ether	-3.60	-3.62		-6.71
ethyl-tert-butylether	CCOC(C)(C)C	diethyl ether	-4.43	-4.06		-7.28
1,4-dioxane	C1COCCO1	diethyl ether	-4.61	-4.76		-8.23
butanone	CCC(C)=O	diethyl ether	-4.13	-4.51		-8.35
acetonitrile	CC#N	diethyl ether	-3.63	-3.94	-7.35	-6.46
trimethylamine	CN(C)C	diethyl ether	-2.36	-3.22		-5.99
nitromethane	C[N+](=O)[O-]	diethyl ether	-4.22	-3.92	-8.73	-7.81
methanol	CO	diethyl ether	-3.38	-3.68	-8.03	-8.17
toluene	Cc1ccccc1	diethyl ether	-5.07	-5.38	-9.19	-9.64
hexafluorobenzene	Fc1c(F)c(F)c(F)c(F)c1F	diethyl ether	-4.27	-3.98		-8.58
hydrogen	[H][H]	dibutyl ether	1.42	1.17		0.62
nitrogen	N#N	dibutyl ether	0.93	0.99		0.43
butane	CCCC	dibutyl ether	-2.44	-2.39		-5.30
pentane	CCCCC	dibutyl ether	-3.18	-3.15	-6.28	-6.52
hexane	CCCCCC	dibutyl ether	-3.85	-3.93	-7.44	-7.76
heptane	CCCCCCC	dibutyl ether	-4.61	-4.65	-8.62	-8.90
octane	CCCCCCCC	dibutyl ether	-5.25	-5.24	-9.79	-9.76
dichloromethane	ClCCl	dibutyl ether	-3.21	-3.24		-6.58
trichloromethane	ClC(Cl)Cl	dibutyl ether	-4.16	-4.08		-7.89
tetrachloromethane	ClC(Cl)(Cl)Cl	dibutyl ether	-4.16	-4.53		-8.51
1,2-dichloroethane	ClCCCl	dibutyl ether	-4.16	-4.26		-8.18
1-chlorobutane	CCCCCl	dibutyl ether	-4.11	-4.05		-7.88
1-chloropentane	CCCCCCl	dibutyl ether	-4.79	-4.71	-9.12	-8.87
dibromomethane	BrCBr	dibutyl ether	-4.55	-4.22		-8.23
diethyl ether	CCOCC	dibutyl ether	-3.31	-3.39	-6.38	-6.75
dibutyl ether	CCCCOCCCC	dibutyl ether	-5.48	-6.06	-10.76	-10.88
1,4-dioxane	C1COCCO1	dibutyl ether	-4.28	-4.67		-8.74
propanone	CC(C)=O	dibutyl ether	-3.07	-2.89		-5.85
butanone	CCC(C)=O	dibutyl ether	-3.72	-3.70	-7.35	-7.13
heptan-2-one	CCCCCCC(=O)	dibutyl ether	-5.74	-5.63	-10.59	-10.10
heptan-4-one	CCCC(=O)CCC	dibutyl ether	-5.62	-5.71	-10.62	-10.27
cyclopentanone	O=C1CCCC1	dibutyl ether	-4.82	-5.34	-9.29	-10.07
acetonitrile	CC#N	dibutyl ether	-2.89	-2.85	-6.40	-4.87
propylamine	CCCN	dibutyl ether	-2.92	-3.74	-6.75	-7.85
butylamine	CCCCN	dibutyl ether	-3.66	-4.44	-7.88	-9.06
nitromethane	C[N+](=O)[O-]	dibutyl ether	-3.53	-2.87		-6.14
methanol	CO	dibutyl ether	-2.65	-2.96	-7.47	-7.31
ethanol	CCO	dibutyl ether	-3.26	-3.65	-8.44	-8.42
butan-1-ol	CCCCO	dibutyl ether	-4.68	-4.91	-10.74	-10.30
benzene	c1ccccc1	dibutyl ether	-4.11	-4.22	-7.90	-7.95
carbon dioxide	O=C=O	diisopropyl ether	-0.74	-0.20		-1.29
heptane	CCCCCCC	diisopropyl ether	-4.62	-4.84		-9.06
2,3-dimethylbutane	CC(C)C(C)C	diisopropyl ether	-3.70	-3.93		-7.67
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	diisopropyl ether	-4.57	-4.71		-8.78
cyclohexane	C1CCCCC1	diisopropyl ether	-4.16	-4.27		-7.73
1,2-dichloroethane	ClCCCl	diisopropyl ether	-3.88	-4.67		-8.92
1-chlorobutane	CCCCCl	diisopropyl ether	-4.22	-4.42		-8.50

2-chlorobutane	CCC(C)Cl	diisopropyl ether	-3.95	-4.31		-8.33
1-chloro-2-methylpropane	CC(C)CCl	diisopropyl ether	-3.98	-4.33		-8.36
2-chloro-2-methylpropane	CC(C)(C)Cl	diisopropyl ether	-3.54	-3.85		-7.55
1,1,2-trichlorotrifluoroethane	FC(F)(Cl)C(F)(Cl)Cl	diisopropyl ether	-3.49	-4.16		-8.24
diisopropyl ether	CC(C)OC(C)C	diisopropyl ether	-4.01	-4.48		-8.26
dioxane	C1COCCO1	diisopropyl ether	-4.38	-4.80		-8.62
butanone	CCC(C)=O	diisopropyl ether	-3.88	-4.30		-8.21
tert-butyl methyl ketone	CC(C)C(C)=O	diisopropyl ether	-4.29	-4.82		-8.98
methanol	CO	diisopropyl ether	-3.26	-3.50		-8.07
propanol	CCCO	diisopropyl ether	-4.39	-4.78		-10.08
propan-2-ol	CC(C)O	diisopropyl ether	-3.86	-4.49		-9.52
butan-1-ol	CCCCO	diisopropyl ether	-5.14	-5.23		-10.65
2-methylpropan-1-ol	CC(C)CO	diisopropyl ether	-4.94	-5.06		-10.37
butan-2-ol	CCC(C)O	diisopropyl ether	-4.56	-5.10		-10.49
benzene	c1ccccc1	diisopropyl ether	-4.20	-4.80		-8.98
toluene	Cc1ccccc1	diisopropyl ether	-4.87	-5.38		-9.86
hexane	CCCCCC	methyl tert-butyl ether	-4.01	-4.06		-7.72
2-methylpentane	CCCC(C)C	methyl tert-butyl ether	-3.77	-3.94		-7.54
heptane	CCCCCCC	methyl tert-butyl ether	-4.68	-4.74		-8.78
cyclopentane	C1CCCC1	methyl tert-butyl ether	-3.55	-3.47		-6.30
cyclohexane	C1CCCCC1	methyl tert-butyl ether	-4.16	-4.22		-7.50
methylcyclohexane	CC1CCCCC1	methyl tert-butyl ether	-4.80	-4.78		-8.41
1,1,2-trifluorotrifluoroethane	FC(F)(Cl)C(F)(Cl)Cl	methyl tert-butyl ether	-3.62	-4.08		-7.93
methyl tert-butyl ether	COC(C)(C)C	methyl tert-butyl ether	-3.81	-3.57		-6.59
dimethyl carbonate	COC(=O)OC	methyl tert-butyl ether	-4.24	-4.64		-8.43
acetonitrile	CC#N	methyl tert-butyl ether	-3.67	-3.95		-6.50
methanol	CO	methyl tert-butyl ether	-3.45	-3.77		-8.45
ethanol	CCO	methyl tert-butyl ether	-3.94	-4.41		-9.49
propan-2-ol	CC(C)O	methyl tert-butyl ether	-4.22	-4.74		-9.88
butan-1-ol	CCCCO	methyl tert-butyl ether	-5.32	-5.48		-11.01
2-methylpropan-2-ol	CC(C)(C)O	methyl tert-butyl ether	-4.37	-4.53		-9.37
benzene	c1ccccc1	methyl tert-butyl ether	-4.31	-4.83		-8.87
n-methylpiperidine	CN1CCCCC1	methyl tert-butyl ether	-4.80	-5.48		-9.40
1,2-dichloroethane	ClCCCl	methyl tert-butyl ether	-4.35	-4.73		-8.83
nitrogen	N#N	dipropyl ether	0.91	0.94		0.46
cyclohexane	C1CCCCC1	dipropyl ether	-4.12	-4.17		-7.67
methanol	CO	dipropyl ether	-2.94	-3.30		-7.81
ethanol	CCO	dipropyl ether	-3.45	-3.99		-8.94
propan-1-ol	CCCO	dipropyl ether	-4.20	-4.66		-9.97
propan-2-ol	CC(C)O	dipropyl ether	-3.74	-4.37		-9.41
2-methylpropan-1-ol	CC(C)CO	dipropyl ether	-4.78	-4.94		-10.25
2-methylpropan-2-ol	CC(C)(C)O	dipropyl ether	-3.92	-4.23		-9.02
tetrachloromethane	ClC(Cl)(Cl)Cl	dipropyl ether	-4.25	-4.78		-8.92
dipropyl ether	CCCOCC	dipropyl ether	-4.54	-4.89		-9.06
1-chlorobutane	CCCCCl	dipropyl ether	-4.23	-4.13		-7.96
dibromomethane	BrCBr	dipropyl ether	-4.58	-4.11		-7.91
helium	[He]	tetrahydrofuran	2.22	2.13	1.94	2.25
krypton	[Kr]	tetrahydrofuran	0.10	0.08	-0.81	-0.62
xenon	[Xe]	tetrahydrofuran	-0.79	-0.97	-2.12	-2.31
hydrogen	[H][H]	tetrahydrofuran	1.46	1.33	1.07	0.88
oxygen	O=O	tetrahydrofuran	0.82	0.81		0.21
nitrogen	N#N	tetrahydrofuran	1.13	0.85	0.32	0.64
carbon dioxide	O=C=O	tetrahydrofuran	-1.12	-0.88	-4.07	-2.58
sulfur dioxide	O=[S]=O	tetrahydrofuran	-3.93	-3.50	-9.39	-7.67
sulfur hexafluoride	F[S](F)(F)(F)(F)F	tetrahydrofuran	0.05	0.46	1.15	-0.51
methane	C	tetrahydrofuran	0.25	0.04	-0.72	-0.90
ethane	CC	tetrahydrofuran	-0.85	-0.84	-3.28	-2.28
hexane	CCCCCC	tetrahydrofuran	-3.87	-3.76	-6.79	-6.92
2-methylpentane	CCCC(C)C	tetrahydrofuran	-3.68	-3.63		-6.72
heptane	CCCCCCC	tetrahydrofuran	-4.56	-4.44	-7.98	-7.98
2,5-dimethylhexane	CC(C)CCC(C)C	tetrahydrofuran	-4.82	-4.77		-8.45
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	tetrahydrofuran	-4.90	-4.56		-8.17
nonane	CCCCCCCCC	tetrahydrofuran	-5.92	-5.76	-10.07	-10.01
cyclohexane	C1CCCCC1	tetrahydrofuran	-4.27	-3.97	-7.02	-6.78
ethylcyclohexane	CCC1CCCCC1	tetrahydrofuran	-5.35	-5.12		-8.52
ethene	C=C	tetrahydrofuran	-0.82	-1.46	-2.73	-3.44
fluoroethane	CCF	tetrahydrofuran	-1.79	-2.01		-4.15
tetrafluoromethane	FC(F)(F)F	tetrahydrofuran	1.00	0.93		0.26
1-chloropentane	CCCCCl	tetrahydrofuran	-5.67	-4.91		-8.75
dichloromethane	ClCCl	tetrahydrofuran	-4.27	-3.86	-8.17	-7.18
trichloromethane	ClC(Cl)Cl	tetrahydrofuran	-5.13	-4.80	-9.47	-8.74
tetrachloromethane	ClC(Cl)(Cl)Cl	tetrahydrofuran	-4.65	-4.83	-8.54	-8.63
1,2-dichloroethane	ClCCCl	tetrahydrofuran	-5.01	-4.70		-8.36
2-chloro-2-methylpropane	CC(C)(C)Cl	tetrahydrofuran	-3.41	-3.80		-7.01
tetrachloroethene	ClC(Cl)=C(Cl)Cl	tetrahydrofuran	-5.43	-5.25	-9.72	-9.37
2-bromo-2-methylpropane	CC(C)(C)Br	tetrahydrofuran	-3.87	-4.16		-7.65
CF <sub>3</sub> CHBrCl	C(F)(F)(F)C(Br)(Cl)	tetrahydrofuran	-5.01	-4.07		-7.59
1,1,2-trifluorotrifluoroethane	FC(F)(Cl)C(F)(Cl)Cl	tetrahydrofuran	-3.37	-3.76		-7.36
1,2-difluorotetrachloroethane	FC(Cl)(Cl)C(F)(Cl)Cl	tetrahydrofuran	-4.82	-5.24		-9.68
diethyl ether	CCOCC	tetrahydrofuran	-3.51	-3.56		-6.31
tetrahydrofuran	C1CCOC1	tetrahydrofuran	-4.28	-3.93	-7.65	-6.65
1,4-dioxane	C1COCCO1	tetrahydrofuran	-5.10	-4.98		-8.42
propionaldehyde	CCC=O	tetrahydrofuran	-3.82	-4.01		-7.24

butyraldehyde	CCCC=O	tetrahydrofuran	-4.42	-4.68		-8.31
propanone	CC(C)=O	tetrahydrofuran	-3.89	-3.97		-7.30
ethyl acetate	CCOC(C)=O	tetrahydrofuran	-4.56	-4.75		-8.40
methyl propanoate	CCC(=O)OC	tetrahydrofuran	-4.45	-4.66		-8.17
acetonitrile	CC#N	tetrahydrofuran	-4.30	-4.61	-8.05	-7.45
triethylamine	CCN(CC)CC	tetrahydrofuran	-4.60	-4.50	-7.96	-8.40
nitromethane	C[N+](=O)=O	tetrahydrofuran	-5.01	-4.77		-9.11
dimethylformamide	CN(C)C=O	tetrahydrofuran	-5.99	-6.27	-10.83	-11.51
methanol	CO	tetrahydrofuran	-3.87	-3.91	-8.10	-8.49
propan-1-ol	CCCO	tetrahydrofuran	-5.18	-5.28		-10.72
tetramethylstannane	C[Sn](C)(C)C	tetrahydrofuran	-3.64	-4.09	-7.20	-6.63
benzene	c1ccccc1	tetrahydrofuran	-4.75	-4.78	-8.42	-8.48
ethylbenzene	CCc1ccccc1	tetrahydrofuran	-6.04	-6.07		-10.49
propylbenzene	CCCc1ccccc1	tetrahydrofuran	-6.64	-6.71		-11.44
isopropylbenzene	CC(C)c1ccccc1	tetrahydrofuran	-6.51	-6.66		-11.39
fluorobenzene	Fc1ccccc1	tetrahydrofuran	-4.94	-4.90	-8.99	-8.66
hexafluorobenzene	Fc1c(F)c(F)c(F)c(F)c1F	tetrahydrofuran	-4.50	-3.62	-8.48	-7.94
1,2-dichlorobenzene	Clc1ccccc1Cl	tetrahydrofuran	-7.11	-7.12		-12.20
hexachlorobenzene	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	tetrahydrofuran	-11.04	-10.18		-17.12
piperidine	C1CCNCC1	tetrahydrofuran	-5.22	-6.00		-10.70
dibutyl ether	CCCCOCCCC	tetrahydrofuran	-6.13	-5.90	-10.55	-9.84
water	O	tetrahydrofuran	-3.97	-4.07	-9.50	-9.48
octane	CCCCCCCC	bis(2-ethoxyethyl) ether	-4.67	-4.56		-8.72
methyl ethyl ketone	CCC(C)=O	bis(2-ethoxyethyl) ether	-4.16	-4.29		-8.82
ethanol	CCO	bis(2-ethoxyethyl) ether	-4.13	-3.38		-8.26
toluene	Cc1ccccc1	bis(2-ethoxyethyl) ether	-4.98	-4.90		-9.39
1,4-dioxane	C1COCCO1	bis(2-ethoxyethyl) ether	-4.78	-4.66		-8.89
neon	[Ne]	tetrahydropyran	2.05	1.95		1.89
argon	[Ar]	tetrahydropyran	0.78	0.73		0.07
krypton	[Kr]	tetrahydropyran	0.11	0.13		-0.59
xenon	[Xe]	tetrahydropyran	-0.79	-0.90		-2.30
hydrogen	[H][H]	tetrahydropyran	1.52	1.35		0.88
deuterium	[H][H]	tetrahydropyran	1.52	1.35		0.88
nitrogen	N#N	tetrahydropyran	1.17	0.88		0.60
tetrafluoromethane	FC(F)(F)F	tetrahydropyran	1.00	0.97		0.23
methane	C	tetrahydropyran	0.28	0.18		-0.69
ethane	CC	tetrahydropyran	-0.87	-0.76		-2.18
ethene	C=C	tetrahydropyran	-0.77	-1.31		-3.23
propane	CCC	tetrahydropyran	-1.66	-1.52		-3.42
propene	CC=C	tetrahydropyran	-1.72	-1.99		-4.26
butane	CCCC	tetrahydropyran	-2.44	-2.33		-4.74
2-methylpropane	CC(C)C	tetrahydropyran	-2.21	-2.21		-4.54
1-butene	CCC=C	tetrahydropyran	-2.50	-2.68		-5.37
trans-2-butene	C/C=C/C	tetrahydropyran	-2.62	-2.67		-5.33
cis-2-butene	C/C=C/C	tetrahydropyran	-2.70	-2.63		-5.23
dimethyl ether	COC	tetrahydropyran	-2.21	-2.44		-4.70
chloroethane	CCCl	tetrahydropyran	-3.08	-2.98		-5.85
1,1-difluoroethane	CC(F)F	tetrahydropyran	-1.98	-2.33		-4.62
hexane	CCCCCC	tetrahydropyran	-3.55	-3.81		-7.09
sulfur hexafluoride	F[S](F)(F)(F)(F)F	tetrahydropyran	0.05	0.27		-1.08
tetrafluoromethane	FC(F)(F)F	tetrahydropyran	1.00	0.97		0.23
helium	[He]	anisole	2.46	2.14		2.26
argon	[Ar]	anisole	1.11	0.93		0.29
krypton	[Kr]	anisole	0.44	0.35		-0.37
methane	C	anisole	0.61	0.14		-0.89
hexane	CCCCCC	anisole	-3.37	-3.32		-6.14
heptane	CCCCCCC	anisole	-4.03	-4.06		-7.35
octane	CCCCCCCC	anisole	-4.68	-4.69		-8.38
2-methylpentane	CCCC(C)C	anisole	-3.16	-3.23		-6.04
2,4-dimethylpentane	CC(C)CC(C)C	anisole	-3.54	-3.86		-7.13
2,5-dimethylhexane	CC(C)CCC(C)C	anisole	-4.19	-4.63		-8.38
2,3,4-trimethylpentane	CC(C)C(C)(C)C	anisole	-4.32	-4.46		-8.23
cyclohexane	C1CCCCC1	anisole	-3.80	-3.67		-6.27
ethylcyclohexane	CCC1CCCCC1	anisole	-4.89	-5.01		-8.43
pent-1-ene	CCCC=C	anisole	-2.78	-2.88		-5.47
3-methyl-1-butene	CC(C)C=C	anisole	-2.62	-2.77		-5.30
trichloromethane	ClC(Cl)Cl	anisole	-4.25	-4.40		-8.08
dichloromethane	ClCCl	anisole	-3.69	-3.38		-6.28
chloropropane	CCCCl	anisole	-3.60	-3.47		-6.51
1,2-dichloroethane	ClCCCl	anisole	-4.57	-4.34		-7.71
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	anisole	-4.18	-5.63		-9.96
iodomethane	CI	anisole	-3.50	-3.31		-5.94
ethyl iodide	CCI	anisole	-4.16	-3.95		-6.95
benzene	c1ccccc1	anisole	-4.41	-4.23		-7.56
toluene	Cc1ccccc1	anisole	-5.14	-4.95		-8.68
1,4-dioxane	C1COCCO1	anisole	-5.08	-4.76		-8.38
nitromethane	C[N+](=O)=O	anisole	-4.59	-4.61		-9.03
methanol	CO	anisole	-2.85	-3.38		-7.63
ethanol	CCO	anisole	-3.45	-3.91		-8.50
1-propanol	CCCO	anisole	-4.15	-4.62		-9.63
1-butanol	CCCCO	anisole	-4.78	-5.26		-10.68
1-pentanol	CCCCCO	anisole	-5.47	-5.78		-11.44
1-hexanol	CCCCCCO	anisole	-6.05	-6.83		-13.19

2-butanol	CCC(C)O	anisole	-4.37	-4.88		-9.94
isobutanol	CC(C)CO	anisole	-4.44	-5.17		-10.51
cyclohexanol	OC1CCCCC1	anisole	-6.61	-6.90		-12.89
2-chloroethanol	OCCCl	anisole	-4.99	-6.52		-12.89
carbon disulfide	S=C=S	anisole	-3.36	-3.43		-4.54
acetonitrile	CC#N	anisole	-3.98	-3.75		-5.95
butanone	CCC(C)=O	anisole	-4.49	-4.11		-7.46
argon	[Ar]	N-methyl-2-pyrrolidone	1.35	1.26		0.48
hydrogen	[H][H]	N-methyl-2-pyrrolidone	1.98	1.70		1.26
nitrogen	N#N	N-methyl-2-pyrrolidone	1.71	1.13		-0.01
carbon dioxide	O=C=O	N-methyl-2-pyrrolidone	-0.86	-0.48	-3.56	-3.06
hydrogen sulfide	S	N-methyl-2-pyrrolidone	-2.25	-1.98		-4.27
COS	O=C=S	N-methyl-2-pyrrolidone	-1.41	-1.70	-3.61	-4.03
ammonia	N	N-methyl-2-pyrrolidone	-1.83	-2.47		-6.28
methane	C	N-methyl-2-pyrrolidone	0.82	0.46	-0.53	-1.23
ethane	CC	N-methyl-2-pyrrolidone	-0.31	-0.17		-2.10
propane	CCC	N-methyl-2-pyrrolidone	-0.89	-0.76	-3.03	-2.92
isobutane	CC(C)C	N-methyl-2-pyrrolidone	-1.20	-1.19		-3.54
n-pentane	CCCCC	N-methyl-2-pyrrolidone	-2.17	-1.88		-4.60
2-methylbutane	CCC(C)C	N-methyl-2-pyrrolidone	-1.80	-1.69	-4.30	-4.27
n-hexane	CCCCCC	N-methyl-2-pyrrolidone	-2.71	-2.45		-5.49
2-methylpentane	CCCC(C)C	N-methyl-2-pyrrolidone	-2.54	-2.21		-5.07
n-heptane	CCCCCCC	N-methyl-2-pyrrolidone	-3.19	-3.03		-6.39
2,2-dimethylpentane	CCCC(C)(C)C	N-methyl-2-pyrrolidone	-2.66	-2.54	-5.19	-5.76
2,4-dimethylpentane	CC(C)CC(C)C	N-methyl-2-pyrrolidone	-2.78	-2.51	-6.11	-5.55
octane	CCCCCCCC	N-methyl-2-pyrrolidone	-3.78	-3.52	-7.34	-7.26
2,5-dimethylhexane	CC(C)CCCC(C)C	N-methyl-2-pyrrolidone	-3.41	-3.08		-6.45
2,3,4-trimethylpentane	CC(C)C(C)(C)C(C)C	N-methyl-2-pyrrolidone	-3.59	-2.76		-6.00
decane	CCCCCCCCC	N-methyl-2-pyrrolidone	-4.92	-4.92		-9.46
cyclopentane	C1CCCC1	N-methyl-2-pyrrolidone	-2.70	-2.68	-5.40	-5.84
methylcyclopentane	CC1CCCC1	N-methyl-2-pyrrolidone	-2.99	-3.02	-6.24	-6.28
cyclohexane	C1CCCCC1	N-methyl-2-pyrrolidone	-3.25	-3.19	-6.34	-6.57
ethylcyclohexane	CCC1CCCCC1	N-methyl-2-pyrrolidone	-4.19	-4.07		-7.88
propylcyclohexane	CCCC1CCCCC1	N-methyl-2-pyrrolidone	-4.57	-4.72		-8.92
butylcyclohexane	CCCCC1CCCCC1	N-methyl-2-pyrrolidone	-5.09	-5.49		-10.18
ethene	C=C	N-methyl-2-pyrrolidone	-0.40	-0.49		-2.50
2-methylpropene	CC(C)=C	N-methyl-2-pyrrolidone	-1.80	-1.71		-4.31
pent-1-ene	CCCC=C	N-methyl-2-pyrrolidone	-2.25	-2.33		-5.22
hex-1-ene	CCCCC=C	N-methyl-2-pyrrolidone	-2.81	-2.90		-6.09
hept-1-ene	CCCCCC=C	N-methyl-2-pyrrolidone	-3.45	-3.49		-7.04
oct-1-ene	CCCCCCC=C	N-methyl-2-pyrrolidone	-3.97	-4.00		-7.89
3-methylbut-1-ene	CC(C)C=C	N-methyl-2-pyrrolidone	-2.03	-2.24		-5.12
2-methylbut-2-ene	CC=C(C)C	N-methyl-2-pyrrolidone	-2.48	-2.33		-5.26
2-methylpent-2-ene	CCC=C(C)C	N-methyl-2-pyrrolidone	-3.06	-2.88		-6.11
buta-1,3-diene	C=CC=C	N-methyl-2-pyrrolidone	-2.36	-2.19		-5.05
cis-penta-1,3-diene	C\C=C/C=C	N-methyl-2-pyrrolidone	-3.11	-2.80		-5.92
trans-hexa-1,3-diene	CC/C=C/C=C	N-methyl-2-pyrrolidone	-3.67	-3.35		-6.72
hexa-1,5-diene	C=CCCC=C	N-methyl-2-pyrrolidone	-3.23	-3.45		-6.95
cyclopentene	C1CC=CC1	N-methyl-2-pyrrolidone	-2.84	-3.01	-5.00	-6.33
cycloheptene	C1CCCC=CC1	N-methyl-2-pyrrolidone	-4.22	-4.04		-7.79
cyclooctene	C1CCCCC=CC1	N-methyl-2-pyrrolidone	-4.91	-3.97		-7.50
cyclopentadiene	C1C=CC=C1	N-methyl-2-pyrrolidone	-3.33	-3.20		-6.62
cyclohexa-1,3-diene	C1CC=CC=C1	N-methyl-2-pyrrolidone	-3.77	-3.75		-7.31
heptyne	CCCCCCC#C	N-methyl-2-pyrrolidone	-4.15	-4.11		-8.06
fluoroethane	CCF	N-methyl-2-pyrrolidone	-1.86	-1.58		-4.15
dichloromethane	ClCCl	N-methyl-2-pyrrolidone	-4.23	-3.07		-6.44
trichloromethane	ClC(Cl)Cl	N-methyl-2-pyrrolidone	-5.24	-3.99		-8.09
tetrachloromethane	ClC(Cl)(Cl)Cl	N-methyl-2-pyrrolidone	-4.16	-4.00		-8.17
2-chloro-2-methylpropane	CC(C)(C)Cl	N-methyl-2-pyrrolidone	-2.97	-3.20		-6.60
2-bromo-2-methylpropane	CC(C)(C)Br	N-methyl-2-pyrrolidone	-3.44	-3.26		-6.69
iodomethane	CI	N-methyl-2-pyrrolidone	-3.77	-3.22		-6.61
difluoromethane	FCF	N-methyl-2-pyrrolidone	-1.69	-0.86		-2.54
tetrafluoromethane	FC(F)(F)F	N-methyl-2-pyrrolidone	1.80	1.21		-0.14
trichlorofluoromethane	FC(Cl)(Cl)Cl	N-methyl-2-pyrrolidone	-2.56	-2.85		-6.67
dichlorofluoromethane	FC(Cl)Cl	N-methyl-2-pyrrolidone	-1.34	-2.86		-6.28
chlorotrifluoromethane	FC(F)(F)Cl	N-methyl-2-pyrrolidone	0.23	0.34		-1.75
1,1-difluoroethane	CC(F)F	N-methyl-2-pyrrolidone	-2.02	-2.14		-4.72
1,1,1,2-tetrafluoroethane	FCC(F)(F)F	N-methyl-2-pyrrolidone	-1.96	-1.59		-3.02
1-chloro-1,2,2,2-tetrafluoroethane	FC(Cl)C(F)(F)F	N-methyl-2-pyrrolidone	-2.39	-1.81		-4.20
1,2-dichlorotetrafluoroethane	FC(F)(Cl)C(F)(F)Cl	N-methyl-2-pyrrolidone	-1.49	-1.40		-4.44
chloropentafluoroethane	FC(F)(F)C(F)(F)Cl	N-methyl-2-pyrrolidone	0.07	-0.01		-2.12
1,1,1,2,3,3,3-heptafluoropropane	FC(C(F)(F)F)C(F)(F)F	N-methyl-2-pyrrolidone	-0.60	-0.98		-1.27
diethylether	CCOCC	N-methyl-2-pyrrolidone	-2.77	-3.18		-6.65
tetrahydrofuran	C1CCOC1	N-methyl-2-pyrrolidone	-4.04	-3.79		-7.53
dioxane	C1COCCO1	N-methyl-2-pyrrolidone	-4.99	-5.02		-9.63
2-methylpropanal	CC(C)C=O	N-methyl-2-pyrrolidone	-3.79	-3.94		-7.61
pentanal	CCCCC=O	N-methyl-2-pyrrolidone	-4.67	-4.44	-7.95	-8.30
crotonaldehyde	C/C=C/C=O	N-methyl-2-pyrrolidone	-4.99	-4.19	-8.71	-7.91
propanone	CC(C)=O	N-methyl-2-pyrrolidone	-3.97	-3.45		-6.93
butanone	CCC(C)=O	N-methyl-2-pyrrolidone	-4.43	-4.02		-7.74
pentan-2-one	CCCC(C)=O	N-methyl-2-pyrrolidone	-4.73	-4.55		-8.63

pentan-3-one	CCC(=O)CC	<i>N</i> -methyl-2-pyrrolidone	-4.76	-4.54		-8.47
methyl formate	COC=O	<i>N</i> -methyl-2-pyrrolidone	-3.71	-3.44		-6.85
propyl acetate	CCCOC(C)=O	<i>N</i> -methyl-2-pyrrolidone	-4.62	-4.75	-8.69	-9.04
vinyl acetate	CC(=O)OC=C	<i>N</i> -methyl-2-pyrrolidone	-4.16	-4.58	-7.92	-8.54
ethyl propanoate	CCOC(=O)CC	<i>N</i> -methyl-2-pyrrolidone	-4.49	-4.46	-8.82	-8.48
ethyl butanoate	CCCC(=O)OCC	<i>N</i> -methyl-2-pyrrolidone	-4.90	-4.99		-9.43
nitromethane	C[N+](=O)[O-]	<i>N</i> -methyl-2-pyrrolidone	-5.50	-4.54		-8.94
ethanol	CCO	<i>N</i> -methyl-2-pyrrolidone	-4.98	-4.18	-9.37	-9.97
propan-1-ol	CCCO	<i>N</i> -methyl-2-pyrrolidone	-5.72	-4.77		-10.96
propan-2-ol	CC(C)O	<i>N</i> -methyl-2-pyrrolidone	-5.09	-4.57		-10.61
benzene	c1ccccc1	<i>N</i> -methyl-2-pyrrolidone	-4.35	-3.84	-7.38	-7.47
toluene	Cc1ccccc1	<i>N</i> -methyl-2-pyrrolidone	-5.07	-4.45	-9.21	-8.44
thiophene	s1ccccc1	<i>N</i> -methyl-2-pyrrolidone	-4.68	-4.71	-7.76	-9.08
sulfuryl fluoride	F[S](F)(=O)=O	<i>N</i> -methyl-2-pyrrolidone	-0.56	-0.66		-1.86
argon	[Ar]	methylformamide	1.32	1.03		0.33
oxygen	O=O	methylformamide	1.12	0.24		-1.03
<i>n</i> -pentane	CCCCC	methylformamide	-1.80	-2.05		-4.52
2-methylbutane	CCC(C)C	methylformamide	-1.57	-1.89	-4.38	-4.19
<i>n</i> -hexane	CCCCCC	methylformamide	-2.33	-2.42		-5.04
2-methylpentane	CCCC(C)C	methylformamide	-2.24	-2.21		-4.61
<i>n</i> -heptane	CCCCCCC	methylformamide	-2.82	-2.81		-5.58
2,4-dimethylpentane	CC(C)CC(C)C	methylformamide	-2.48	-2.35		-4.76
octane	CCCCCCCC	methylformamide	-3.31	-3.13	-8.39	-6.15
2,5-dimethylhexane	CC(C)CCC(C)C	methylformamide	-2.96	-2.74		-5.35
2,3,4-trimethylpentane	CC(C)(C)C(C)C	methylformamide	-3.22	-2.35		-4.71
methylcyclopentane	CC1CCCC1	methylformamide	-2.67	-3.45	-6.47	-6.65
cyclohexane	C1CCCCC1	methylformamide	-2.91	-3.53	-6.81	-6.78
methylcyclohexane	CC1CCCCC1	methylformamide	-3.18	-3.68	-7.40	-6.87
ethylcyclohexane	CCC1CCCCC1	methylformamide	-3.72	-3.99		-7.23
pent-1-ene	CCCC=C	methylformamide	-1.98	-2.44		-5.13
3-methylbut-1-ene	CC(C)C=C	methylformamide	-1.75	-2.32		-4.82
2-methylbut-2-ene	CC=C(C)C	methylformamide	-2.17	-2.58		-5.39
hex-1-ene	CCCCC=C	methylformamide	-2.55	-2.77		-5.56
oct-1-ene	CCCCCCC=C	methylformamide	-3.60	-3.22		-6.07
2-methylbuta-1,3-diene	CC(=C)C=C	methylformamide	-2.44	-2.94		-5.97
cyclohexene	C1CCC=CC1	methylformamide	-3.26	-3.84	-7.25	-7.36
diethylether	CCOCC	methylformamide	-2.66	-3.18		-6.59
di-isopropylether	CC(C)OC(C)C	methylformamide	-3.04	-3.73		-7.30
methyl t-butyl ether	COC(C)(C)C	methylformamide	-3.08	-3.47		-7.01
methyl t-pentyl ether	CCC(C)(C)OC	methylformamide	-3.62	-3.62		-7.19
ethyl t-butyl ether	CCOC(C)(C)C	methylformamide	-3.21	-3.76		-7.44
1,4-dioxane	C1COCCO1	methylformamide	-4.86	-5.45	-9.02	-10.15
propanone	CC(C)=O	methylformamide	-3.82	-4.11		-8.22
butanone	CCC(C)=O	methylformamide	-4.27	-4.34	-8.13	-8.43
pentan-2-one	CCCC(C)=O	methylformamide	-4.69	-4.78		-9.12
methylformamide	CNC=O	methylformamide	-8.24	-6.69	-13.00	-13.45
water	O	methylformamide	-5.28	-5.30		-12.47
methanol	CO	methylformamide	-4.54	-4.08	-8.38	-9.61
toluene	Cc1ccccc1	methylformamide	-4.34	-4.53	-8.70	-8.47
ethylbenzene	CCc1ccccc1	methylformamide	-4.82	-4.94	-9.66	-9.04
<i>o</i> -xylene	Cc1ccccc1C	methylformamide	-5.02	-5.00		-9.20
<i>m</i> -xylene	Cc1cccc(C)c1	methylformamide	-4.82	-5.06		-9.33
<i>p</i> -xylene	Cc1ccc(C)cc1	methylformamide	-4.80	-5.07		-9.33
argon	[Ar]	<i>n</i> -methylacetamide	1.17	1.10		0.36
nitrogen	N#N	<i>n</i> -methylacetamide	1.53	1.46		0.93
hydrogen sulfide	S	<i>n</i> -methylacetamide	-1.77	-2.49		-5.33
ethane	CC	<i>n</i> -methylacetamide	-0.26	-0.91		-3.08
2-methylbutane	CCC(C)C	<i>n</i> -methylacetamide	-2.03	-1.85		-4.29
<i>n</i> -hexane	CCCCCC	<i>n</i> -methylacetamide	-2.74	-2.38		-5.12
<i>n</i> -heptane	CCCCCCC	<i>n</i> -methylacetamide	-3.34	-2.78		-5.71
cyclohexane	C1CCCCC1	<i>n</i> -methylacetamide	-3.26	-3.49		-6.85
methylcyclohexane	CC1CCCCC1	<i>n</i> -methylacetamide	-3.59	-3.65		-6.94
pent-1-ene	CCCC=C	<i>n</i> -methylacetamide	-2.22	-2.38		-5.16
3-methylbut-1-ene	CC(C)C=C	<i>n</i> -methylacetamide	-2.14	-2.26		-4.85
2-methylbut-2-ene	CC=C(C)C	<i>n</i> -methylacetamide	-2.54	-2.37		-5.10
2-methylbuta-1,3-diene	CC(=C)C=C	<i>n</i> -methylacetamide	-2.74	-2.72		-5.63
<i>cis</i> -penta-1,3-diene	C/C=C/C=C	<i>n</i> -methylacetamide	-2.89	-2.79		-5.80
cyclohexene	C1CCC=CC1	<i>n</i> -methylacetamide	-3.52	-3.76		-7.34
dichloromethane	ClCCl	<i>n</i> -methylacetamide	-3.74	-3.43		-7.18
trichloromethane	ClC(Cl)Cl	<i>n</i> -methylacetamide	-4.57	-3.90		-7.74
tetrachloromethane	ClC(Cl)(Cl)Cl	<i>n</i> -methylacetamide	-3.90	-3.66		-7.25
trichloroethene	ClC=C(Cl)Cl	<i>n</i> -methylacetamide	-4.35	-3.96		-7.86
diethylether	CCOCC	<i>n</i> -methylacetamide	-2.77	-2.97		-6.28
di-isopropylether	CC(C)OC(C)C	<i>n</i> -methylacetamide	-3.25	-3.52		-7.02
methyl t-butyl ether	COC(C)(C)C	<i>n</i> -methylacetamide	-3.12	-3.23		-6.65
methyl t-pentyl ether	CCC(C)(C)OC	<i>n</i> -methylacetamide	-3.75	-3.43		-6.95
isopropyl t-butyl ether	CC(C)OC(C)(C)C	<i>n</i> -methylacetamide	-3.62	-3.82		-7.69
dioxane	C1COCCO1	<i>n</i> -methylacetamide	-4.67	-5.20		-9.73
furan	o1ccccc1	<i>n</i> -methylacetamide	-3.23	-3.98		-7.95
butanone	CCC(C)=O	<i>n</i> -methylacetamide	-4.19	-4.07		-8.01
4-methylpentan-2-one	CC(C)CC(C)=O	<i>n</i> -methylacetamide	-4.82	-4.45		-8.49
ethyl acetate	CCOC(C)=O	<i>n</i> -methylacetamide	-4.04	-4.86		-9.03
butyl acetate	CCCCOC(C)=O	<i>n</i> -methylacetamide	-5.14	-5.38		-9.77

acetonitrile	CC#N	<i>n</i> -methylacetamide	-4.23	-4.03		-7.29
<i>n</i> -methylacetamide	CNC(C)=O	<i>n</i> -methylacetamide	-8.61	-7.08		-14.42
water	O	<i>n</i> -methylacetamide	-5.80	-5.21		-12.46
methanol	CO	<i>n</i> -methylacetamide	-4.72	-3.95		-9.50
propan-2-ol	CC(C)O	<i>n</i> -methylacetamide	-5.12	-4.58		-10.46
butan-1-ol	CCCCO	<i>n</i> -methylacetamide	-6.10	-4.73		-10.61
2-methylpropan-1-ol	CC(C)CO	<i>n</i> -methylacetamide	-5.91	-4.57		-10.32
allyl alcohol	OCC=C	<i>n</i> -methylacetamide	-5.87	-5.26		-11.64
benzene	c1ccccc1	<i>n</i> -methylacetamide	-3.87	-3.71		-7.19
toluene	Cc1ccccc1	<i>n</i> -methylacetamide	-4.57	-4.29		-8.09
pyridine	c1ccncc1	<i>n</i> -methylacetamide	-5.35	-5.38		-9.69
2-methylpropane	CC(C)C	formamide	-1.32	-0.79		-3.80
<i>n</i> -pentane	CCCCC	formamide	-0.44	-1.13		-4.18
octane	CCCCCCCC	formamide	-1.27	-2.61	-7.41	-6.52
nonane	CCCCCCCCC	formamide	-1.66	-3.21	-9.20	-7.44
methylcyclohexane	CC1CCCCC1	formamide	-1.42	-3.01	-6.20	-7.07
ethylcyclohexane	CCC1CCCCC1	formamide	-1.81	-3.39	-7.30	-7.66
propylcyclohexane	CCCC1CCCCC1	formamide	-1.91	-3.72		-8.17
isobutylene	CC(C)=C	formamide	-1.98	-1.06		-4.21
hex-1-ene	CCCCC=C	formamide	-0.91	-2.11		-5.66
hept-1-ene	CCCCC=C	formamide	-1.24	-2.63		-6.41
oct-1-ene	CCCCC=C	formamide	-1.58	-3.05		-7.04
<i>cis</i> -hex-2-ene	CCC/C=C/C	formamide	-1.06	-2.09		-5.60
cyclohexene	C1CCC=CC1	formamide	-1.87	-2.80	-6.30	-6.63
dichloromethane	ClCCl	formamide	-2.67	-2.62		-6.76
trichloromethane	ClC(Cl)Cl	formamide	-2.91	-3.28		-7.85
tetrachloromethane	ClC(Cl)(Cl)Cl	formamide	-2.17	-3.27		-7.91
diethylether	CCOCC	formamide	-2.03	-2.53		-6.50
tetrahydrofuran	C1CCOC1	formamide	-3.67	-3.27		-7.55
propanal	CCC=O	formamide	-3.26	-2.81		-6.72
butanal	CCCC=O	formamide	-3.52	-3.34		-7.61
pentanal	CCCCC=O	formamide	-3.77	-3.76		-8.18
octanal	CCCCCCC=O	formamide	-4.31	-4.99		-10.14
nonanal	CCCCCCCC=O	formamide	-4.37	-5.70		-11.10
propanone	CC(C)=O	formamide	-3.72	-3.19		-7.46
butanone	CCC(C)=O	formamide	-3.96	-3.46		-7.80
pentan-2-one	CCCC(C)=O	formamide	-4.12	-3.95		-8.62
hexan-2-one	CCCCC(C)=O	formamide	-4.46	-4.42		-9.33
heptan-2-one	CCCCC(C)=O	formamide	-4.75	-4.75		-9.81
octan-2-one	CCCCC(C)=O	formamide	-5.06	-5.27		-10.55
methyl isobutyl ketone	CC(C)CC(C)=O	formamide	-4.19	-4.26		-9.17
methyl isohexyl ketone	CC(C)CCCC(C)=O	formamide	-5.09	-5.28		-10.60
methyl acetate	CC(=O)OC	formamide	-3.27	-3.81		-8.15
ethyl acetate	CC(=O)OCC	formamide	-3.56	-4.09		-8.60
propyl acetate	CC(=O)OCC	formamide	-3.72	-4.48		-9.31
butyl acetate	CC(=O)OCCC	formamide	-4.07	-4.69		-9.69
pentyl acetate	CC(=O)OCCCC	formamide	-4.32	-4.97		-10.18
hexyl acetate	CC(=O)OCCCCC	formamide	-4.60	-5.30		-10.73
acetonitrile	CC#N	formamide	-4.37	-3.58	-7.80	-7.01
nitromethane	C[N+](=O)[O-]	formamide	-4.75	-4.49		-9.80
formamide	NC=O	formamide	-9.96	-6.72	-14.39	-14.03
water	O	formamide	-5.67	-4.68	-10.23	-12.97
methanol	CO	formamide	-4.50	-3.16	-8.74	-9.35
propan-1-ol	CCCO	formamide	-4.84	-4.20		-11.10
butan-1-ol	CCCCO	formamide	-5.22	-4.52	-11.59	-11.54
hexan-1-ol	CCCCCO	formamide	-6.04	-5.48	-13.16	-13.05
octan-1-ol	CCCCCCCO	formamide	-6.49	-6.61	-15.06	-14.76
nonan-1-ol	CCCCCCCCO	formamide	-7.22	-7.14		-15.56
toluene	Cc1ccccc1	formamide	-3.00	-3.70	-8.01	-8.01
propylbenzene	CCCc1ccccc1	formamide	-3.49	-4.77	-9.20	-9.57
isopropylbenzene	CC(C)c1ccccc1	formamide	-3.38	-4.68	-8.80	-9.45
<i>o</i> -xylene	Cc1ccccc1C	formamide	-3.55	-4.17	-8.80	-8.76
<i>m</i> -xylene	Cc1ccc(C)cc1	formamide	-3.29	-4.22	-8.39	-8.81
<i>p</i> -xylene	Cc1ccc(C)cc1	formamide	-3.27	-4.23	-8.39	-8.82
fluorobenzene	Fc1ccccc1	formamide	-2.80	-3.63	-7.46	-8.03
chlorobenzene	Clc1ccccc1	formamide	-3.57	-4.66	-8.77	-9.60
bromobenzene	Brc1ccccc1	formamide	-4.12	-4.98	-9.63	-10.04
1,2-dichlorobenzene	Clc1ccccc1Cl	formamide	-4.54	-5.74		-11.43
naphthalene	c1ccc2ccccc2c1	formamide	-5.47	-6.24	-11.83	-12.00
oxygen	O=O	ethylbenzene	0.84	0.87		0.31
chlorine	ClCl	ethylbenzene	-2.19	-1.36		-3.03
carbon dioxide	O=C=O	ethylbenzene	-0.46	-0.39		-1.88
propane	CCC	ethylbenzene	-1.62	-1.42		-3.10
heptane	CCCCCCC	ethylbenzene	-4.50	-4.38		-7.80
decane	CCCCCCCCC	ethylbenzene	-6.58	-6.65		-11.44
cyclohexane	C1CCCCC1	ethylbenzene	-4.10	-4.09		-7.15
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	ethylbenzene	-4.35	-4.61		-8.34
tetrachloromethane	ClC(Cl)(Cl)Cl	ethylbenzene	-4.24	-4.35		-7.68
1-chlorohexane	CCCCC(Cl)C	ethylbenzene	-5.77	-5.54		-9.69
tetrahydrofuran	C1CCOC1	ethylbenzene	-4.17	-4.05		-7.30
1,4-dioxane	C1CCOCCO1	ethylbenzene	-4.71	-4.67		-8.33
acetone	CC(C)=O	ethylbenzene	-3.42	-3.25		-6.07
butanone	CCC(C)=O	ethylbenzene	-4.12	-3.97		-7.21

2-pentanone	CCCC(C)=O	ethylbenzene	-4.85	-4.73		-8.43
2-heptanone	CCCCC(C)=O	ethylbenzene	-6.12	-6.08		-10.56
methanol	CO	ethylbenzene	-2.32	-2.01		-4.45
ethanol	CCO	ethylbenzene	-3.02	-2.68		-5.61
2-methyl-isopropanol	CC(C)(C)O	ethylbenzene	-3.50	-3.85		-7.77
butan-2-ol	CCC(C)O	ethylbenzene	-4.08	-4.05		-7.90
3-methyl-1-butanol	CC(C)CCO	ethylbenzene	-4.88	-4.86		-9.14
hexan-1-ol	CCCCCCO	ethylbenzene	-5.90	-5.65		-10.51
heptan-1-ol	CCCCCCCO	ethylbenzene	-6.87	-6.46		-11.85
2-chloroethanol	OCCCl	ethylbenzene	-4.65	-4.66		-8.61
benzene	c1ccccc1	ethylbenzene	-4.34	-4.24		-7.66
toluene	Cc1ccccc1	ethylbenzene	-5.08	-5.01		-8.88
ethylbenzene	CCc1ccccc1	ethylbenzene	-5.73	-5.76		-10.03
butylamine	CCCCN	ethylbenzene	-4.11	-3.99		-7.66
ethylamine	CCN	ethylbenzene	-2.59	-2.54		-5.10
diethylamine	CCNCC	ethylbenzene	-3.88	-3.88		-7.83
chlorobenzene	Clc1ccccc1	ethylbenzene	-5.58	-5.55		-9.67
2-furaldehyde	O=Cc1occc1	ethylbenzene	-5.86	-5.27		-9.41
helium	[He]	m-xylene	2.31	2.00		1.99
neon	[Ne]	m-xylene	2.03	1.84		1.66
argon	[Ar]	m-xylene	0.86	0.68		-0.01
krypton	[Kr]	m-xylene	0.19	0.08		-0.84
hydrogen	[H][H]	m-xylene	1.49	1.60		1.28
oxygen	O=O	m-xylene	0.85	0.87		0.27
nitric oxide	[N]=O	m-xylene	0.79	0.47		-0.26
carbon dioxide	O=C=O	m-xylene	-0.45	-0.36		-1.88
methane	C	m-xylene	0.37	0.23		-0.56
propane	CCC	m-xylene	-1.62	-1.39		-3.10
butane	CCCC	m-xylene	-2.34	-2.09		-4.18
pentane	CCCCC	m-xylene	-3.11	-2.83		-5.36
hexane	CCCCCC	m-xylene	-3.85	-3.59		-6.58
1-butene	CCC=C	m-xylene	-2.30	-2.20		-4.35
cis-2-butene	C/C=C/C	m-xylene	-2.57	-2.28		-4.53
2-methylprop-1-ene	CC(C)=C	m-xylene	-2.33	-2.13		-4.25
1,3-butadiene	C=CC=C	m-xylene	-2.48	-2.31		-4.54
tetrafluoromethane	FC(F)(F)F	m-xylene	1.13	1.21		0.49
difluoromethane	FCF	m-xylene	-0.83	-0.75		-2.07
trifluoromethane	FC(F)F	m-xylene	-0.29	-0.22		-1.39
chloroethane	CCCl	m-xylene	-2.87	-2.54		-4.92
dichloromethane	ClCCl	m-xylene	-3.58	-3.05		-5.66
tetrachloromethane	ClC(Cl)(Cl)Cl	m-xylene	-4.29	-4.31		-7.67
1,2-dichloroethane	ClCCCl	m-xylene	-4.45	-4.12		-7.33
1,1-difluoroethane	CC(F)F	m-xylene	-1.63	-1.56		-3.26
1,1,2-trichlorotrifluoroethane	FC(F)(Cl)C(F)(Cl)Cl	m-xylene	-3.37	-3.10		-6.22
diethyl ether	CCOCC	m-xylene	-3.29	-3.35		-6.21
propanone	CC(C)=O	m-xylene	-3.40	-3.20		-6.04
butanone	CCC(C)=O	m-xylene	-4.09	-3.93		-7.20
2-pentanone	CCCC(C)=O	m-xylene	-4.86	-4.69		-8.42
2-hexanone	CCCCC(C)=O	m-xylene	-5.47	-5.39		-9.52
2-heptanone	CCCCC(C)=O	m-xylene	-6.19	-6.07		-10.59
methanol	CO	m-xylene	-2.42	-1.95		-4.40
ethanol	CCO	m-xylene	-3.00	-2.62		-5.56
butan-1-ol	CCCCO	m-xylene	-4.38	-4.11		-8.00
propan-2-ol	CC(C)O	m-xylene	-3.33	-3.26		-6.60
2-methylpropan-1-ol	CC(C)CO	m-xylene	-4.10	-3.95		-7.74
3-methyl-1-butanol	CC(C)CCO	m-xylene	-4.93	-4.82		-9.10
2-chloroethanol	OCCCl	m-xylene	-4.69	-4.57		-8.46
benzene	c1ccccc1	m-xylene	-4.34	-4.20		-7.64
m-xylene	Cc1ccc(C)c1	m-xylene	-5.80	-5.71		-10.05
helium	[He]	o-xylene	2.35	2.00		1.98
neon	[Ne]	o-xylene	2.13	1.85		1.67
argon	[Ar]	o-xylene	0.90	0.71		0.02
krypton	[Kr]	o-xylene	0.23	0.11		-0.83
oxygen	O=O	o-xylene	0.88	0.81		0.12
carbon dioxide	O=C=O	o-xylene	-0.43	-0.41		-2.04
tetrafluoromethane	FC(F)(F)F	o-xylene	1.21	1.24		0.49
sulfur hexafluoride	F[S](F)(F)(F)(F)F	o-xylene	0.27	0.53		-0.71
methane	C	o-xylene	0.40	0.22		-0.63
propane	CCC	o-xylene	-1.52	-1.35		-3.05
butane	CCCC	o-xylene	-2.31	-2.04		-4.13
2-methylpropane	CC(C)C	o-xylene	-2.04	-1.94		-3.96
1-propene	CC=C	o-xylene	-1.56	-1.48		-3.25
1-butene	CCC=C	o-xylene	-2.31	-2.18		-4.34
cis-2-butene	C/C=C/C	o-xylene	-2.54	-2.26		-4.51
2-methylprop-1-ene	CC(C)=C	o-xylene	-2.31	-2.15		-4.33
1,3-butadiene	C=CC=C	o-xylene	-2.46	-2.31		-4.55
chloroethane	CCCl	o-xylene	-2.86	-2.54		-4.95
dichloromethane	ClCCl	o-xylene	-3.58	-3.11		-5.80
tetrachloromethane	ClC(Cl)(Cl)Cl	o-xylene	-4.34	-4.34		-7.75
1,2-dichloroethane	ClCCCl	o-xylene	-4.42	-4.19		-7.47
propanone	CC(C)=O	o-xylene	-3.36	-3.33		-6.29
butan-1-ol	CCCCO	o-xylene	-4.46	-4.20		-8.23
1-hexanol	CCCCCCO	o-xylene	-5.91	-5.82		-10.83

chlorobenzene	Clc1ccccc1	<i>o</i> -xylene	-5.59	-5.55		-9.75
helium	[He]	<i>p</i> -xylene	2.28	2.00		1.99
neon	[Ne]	<i>p</i> -xylene	2.07	1.84		1.66
argon	[Ar]	<i>p</i> -xylene	0.83	0.67		-0.02
krypton	[Kr]	<i>p</i> -xylene	0.17	0.07		-0.84
carbon dioxide	O=C=O	<i>p</i> -xylene	-0.45	-0.33		-1.82
tetrafluoromethane	FC(F)(F)F	<i>p</i> -xylene	1.11	1.21		0.50
methane	C	<i>p</i> -xylene	0.33	0.23		-0.56
propane	CCC	<i>p</i> -xylene	-1.56	-1.41		-3.12
butane	CCCC	<i>p</i> -xylene	-2.33	-2.10		-4.20
2-methylpropane	CC(C)C	<i>p</i> -xylene	-2.06	-2.00		-4.05
pentane	CCCCC	<i>p</i> -xylene	-3.14	-2.85		-5.39
hexane	CCCCCC	<i>p</i> -xylene	-3.84	-3.62		-6.61
heptane	CCCCCCC	<i>p</i> -xylene	-4.55	-4.38		-7.85
octane	CCCCCCCC	<i>p</i> -xylene	-5.24	-5.12		-9.08
nonane	CCCCCCCCC	<i>p</i> -xylene	-5.91	-5.89		-10.27
decane	CCCCCCCCC	<i>p</i> -xylene	-6.68	-6.66		-11.50
octacosane	CCCCCCCCCCCCCCCCCCCCCCCC	<i>p</i> -xylene	-19.33	-17.31		-28.31
2-methylpentane	CCCC(C)C	<i>p</i> -xylene	-3.62	-3.49		-6.40
2,4-dimethylpentane	CC(C)CC(C)C	<i>p</i> -xylene	-4.04	-4.10		-7.39
2,5-dimethylhexane	CC(C)CCC(C)C	<i>p</i> -xylene	-4.74	-4.87		-8.62
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	<i>p</i> -xylene	-4.83	-4.65		-8.28
cyclohexane	C1CCCCC1	<i>p</i> -xylene	-4.18	-4.09		-7.22
ethylcyclohexane	CCC1CCCCC1	<i>p</i> -xylene	-5.32	-5.47		-9.40
1-propene	CC=C	<i>p</i> -xylene	-1.58	-1.49		-3.25
1-butene	CCC=C	<i>p</i> -xylene	-2.33	-2.20		-4.35
<i>cis</i> -2-butene	C/C=C/C	<i>p</i> -xylene	-2.55	-2.28		-4.52
1,3-butadiene	C=CC=C	<i>p</i> -xylene	-2.45	-2.29		-4.52
isopentene	CC(C)C=C	<i>p</i> -xylene	-3.31	-2.76		-5.21
pent-1-ene	CCCC=C	<i>p</i> -xylene	-3.11	-2.90		-5.45
vinylacetylene	C=CC#C	<i>p</i> -xylene	-3.07	-2.31		-4.64
chloroethane	CCCl	<i>p</i> -xylene	-2.83	-2.52		-4.89
dichloromethane	ClCCl	<i>p</i> -xylene	-3.55	-3.02		-5.60
tetrachloromethane	ClC(Cl)(Cl)Cl	<i>p</i> -xylene	-4.35	-4.31		-7.65
1-chloropropane	CCCCl	<i>p</i> -xylene	-3.58	-3.36		-6.25
2-chloro-2-methylpropane	CC(C)(C)Cl	<i>p</i> -xylene	-3.58	-3.77		-6.87
1,2-dichloroethane	ClCCCl	<i>p</i> -xylene	-4.41	-4.09		-7.27
bromoethane	CCBr	<i>p</i> -xylene	-3.41	-3.37		-6.48
iodoethane	CCl	<i>p</i> -xylene	-4.14	-4.10		-7.05
dimethyl ether	COC	<i>p</i> -xylene	-2.03	-2.14		-4.36
1,4-dioxane	C1COCCO1	<i>p</i> -xylene	-4.77	-4.61		-8.30
propanone	CC(C)=O	<i>p</i> -xylene	-3.39	-3.13		-5.92
butanone	CCC(C)=O	<i>p</i> -xylene	-4.22	-3.88		-7.11
2-pentanone	CCCC(C)=O	<i>p</i> -xylene	-4.85	-4.63		-8.33
2-hexanone	CCCCC(C)=O	<i>p</i> -xylene	-5.50	-5.34		-9.43
2-heptanone	CCCCCC(C)=O	<i>p</i> -xylene	-6.18	-6.01		-10.49
triethylamine	CCN(CC)CC	<i>p</i> -xylene	-4.52	-4.44		-8.39
nitromethane	C[N+](=O)=O	<i>p</i> -xylene	-4.09	-3.62		-7.16
ethanol	CCO	<i>p</i> -xylene	-3.03	-2.55		-5.41
propan-1-ol	CCCO	<i>p</i> -xylene	-3.73	-3.35		-6.73
butan-1-ol	CCCCO	<i>p</i> -xylene	-4.49	-4.04		-7.86
propan-2-ol	CC(C)CO	<i>p</i> -xylene	-3.39	-3.20		-6.46
2-methylpropan-1-ol	CC(C)CO	<i>p</i> -xylene	-4.25	-3.89		-7.60
3-methyl-1-butanol	CC(C)CCO	<i>p</i> -xylene	-4.93	-4.76		-8.96
2-chloroethanol	OCCCl	<i>p</i> -xylene	-4.77	-4.45		-8.25
carbon disulfide	S=C=S	<i>p</i> -xylene	-3.55	-3.92		-5.46
toluene	Cc1ccccc1	<i>p</i> -xylene	-5.10	-4.95		-8.83
<i>p</i> -xylene	Cc1ccc(C)cc1	<i>p</i> -xylene	-5.77	-5.70		-10.02
chlorobenzene	Clc1ccccc1	<i>p</i> -xylene	-5.52	-5.48		-9.60
ethyl acetate	CCOC(C)=O	<i>p</i> -xylene	-4.21	-4.06		-7.46
argon	[Ar]	toluene	0.82	0.59	0.23	-0.07
xenon	[Xe]	toluene	-0.72	-0.94	-1.98	-2.28
hydrogen	[H][H]	toluene	1.59	1.50	1.22	1.21
oxygen	O=O	toluene	0.94	0.74	-0.14	0.19
nitrogen	N#N	toluene	1.20	0.92	1.48	0.91
nitric oxide	[N]=O	toluene	0.81	0.33		-0.32
ethane	CC	toluene	-0.75	-0.78	-2.13	-1.99
propane	CCC	toluene	-1.61	-1.51		-3.12
butane	CCCC	toluene	-2.38	-2.20		-4.20
2-methylpropane	CC(C)C	toluene	-2.11	-2.10		-4.04
pentane	CCCCC	toluene	-3.14	-2.96	-5.95	-5.41
hexane	CCCCCC	toluene	-3.85	-3.72	-6.37	-6.62
heptane	CCCCCCC	toluene	-4.55	-4.49	-7.41	-7.86
2,4-dimethylpentane	CC(C)CC(C)C	toluene	-4.04	-4.20		-7.39
octane	CCCCCCCC	toluene	-5.26	-5.22	-8.48	-9.09
2,5-dimethylhexane	CC(C)CCC(C)C	toluene	-4.74	-4.97		-8.61
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	toluene	-4.83	-4.75		-8.28
nonane	CCCCCCCCC	toluene	-5.93	-5.95	-9.48	-10.20
cyclohexane	C1CCCCC1	toluene	-4.17	-4.15	-7.30	-7.09
ethylcyclohexane	CCC1CCCCC1	toluene	-5.34	-5.51		-9.29
ethene	C=C	toluene	-0.69	-0.83	-2.10	-2.04
propene	CC=C	toluene	-1.65	-1.63		-3.32



1-butene	CCC=C	toluene	-2.41	-2.31		-4.37
cis-2-butene	C/C=C/C	toluene	-2.63	-2.43		-4.62
1-pentene	CCCC=C	toluene	-3.11	-2.98		-5.42
hex-1-ene	CCCCC=C	toluene	-3.88	-3.75		-6.64
isobutene	CC(C)=C	toluene	-2.39	-2.33		-4.46
isopentene	CC(C)C=C	toluene	-2.93	-2.88		-5.24
1,3-butadiene	C=CC=C	toluene	-2.55	-2.45		-4.63
2-methylbuta-1,3-diene	CC(=C)C=C	toluene	-3.31	-3.13		-5.75
tetrafluoromethane	FC(F)(F)F	toluene	1.09	1.15	1.43	0.50
fluoromethane	CF	toluene	-0.79	-0.68		-1.86
difluoromethane	FCF	toluene	-0.82	-0.85		-2.07
dichloromethane	CICCl	toluene	-3.64	-3.25		-5.86
tetrachloromethane	ClC(Cl)(Cl)Cl	toluene	-4.33	-4.52		-7.88
chloroethane	CCCl	toluene	-2.97	-2.64		-4.93
1-chloropropane	CCCCl	toluene	-3.66	-3.52		-6.37
1-chlorobutane	CCCCCl	toluene	-4.35	-4.23		-7.50
2-chloro-2-methylpropane	CC(C)(C)Cl	toluene	-3.67	-3.94		-7.06
1-chlorohexane	CCCCCCl	toluene	-5.87	-5.59		-9.63
bromoethane	CCBr	toluene	-3.51	-3.48		-6.51
iodomethane	CI	toluene	-3.51	-3.64		-6.24
1,1-difluoroethane	CC(F)F	toluene	-1.75	-1.81		-3.67
diethyl ether	CCOCC	toluene	-3.33	-3.57	-6.59	-6.46
di-n-butylether	CCCCOCCCC	toluene	-5.96	-6.16		-10.53
methyl t-butyl ether	COC(C)(C)C	toluene	-3.67	-3.96		-7.19
ethyl t-butyl ether	CCOC(C)(C)C	toluene	-4.11	-4.55		-8.13
methyl t-pentyl ether	CCC(C)(C)OC	toluene	-4.50	-4.55		-8.15
tetrahydrofuran	C1CCOC1	toluene	-4.39	-4.32	-8.07	-7.77
1,4-dioxane	C1COCCO1	toluene	-4.93	-4.94	-9.16	-8.76
butanal	CCCC=O	toluene	-4.00	-4.05		-7.20
propanone	CC(C)=O	toluene	-3.52	-3.49		-6.48
butanone	CCC(C)=O	toluene	-4.29	-4.22		-7.63
hexan-2-one	CCCCC(C)=O	toluene	-5.60	-5.56		-9.70
3,3-dimethylbutan-2-one	CC(=O)C(C)(C)C	toluene	-5.00	-5.03		-8.88
methyl acetate	COC(C)=O	toluene	-3.63	-3.95		-7.27
ethyl acetate	CCOC(C)=O	toluene	-4.32	-4.40	-8.34	-7.96
propyl acetate	CCCOC(C)=O	toluene	-5.00	-5.13	-9.39	-9.13
butyl acetate	CCCCOC(C)=O	toluene	-5.57	-5.78	-10.57	-10.18
pentyl acetate	CCCCCOC(C)=O	toluene	-6.41	-6.41		-11.18
methyl propanoate	CCC(=O)OC	toluene	-4.62	-4.39	-8.46	-7.88
methyl pentanoate	CCCCC(=O)OC	toluene	-5.65	-5.80		-10.17
methyl hexanoate	CCCCCC(=O)OC	toluene	-6.38	-6.48		-11.22
propionitrile	CCC#N	toluene	-4.29	-4.24		-6.96
methylamine	CN	toluene	-2.65	-1.86		-3.62
n-propylamine	CCCN	toluene	-3.52	-3.09		-6.12
n-butylamine	CCCCN	toluene	-4.43	-3.90		-7.41
diethylamine	CCNCC	toluene	-3.75	-3.96		-7.79
dipropylamine	CCCNCCC	toluene	-5.24	-5.22		-10.01
trimethylamine	CN(C)C	toluene	-2.71	-2.93		-5.70
triethylamine	CCN(CC)CC	toluene	-4.71	-4.59	-8.27	-8.49
nitromethane	C[N+](=O)[O-]	toluene	-4.22	-3.93		-7.68
nitropropane	CCC[N+](=O)[O-]	toluene	-5.25	-5.32		-9.86
methanol	CO	toluene	-2.42	-2.05	-5.54	-4.36
ethanol	CCO	toluene	-3.00	-2.72	-6.67	-5.53
propan-1-ol	CCCO	toluene	-3.75	-3.53		-6.87
butan-2-ol	CCC(C)O	toluene	-4.20	-4.12		-7.85
2-methylpropan-1-ol	CC(C)CO	toluene	-4.21	-4.06		-7.73
2-methylpropan-2-ol	CC(C)(C)O	toluene	-3.74	-3.92		-7.75
pentan-1-ol	CCCCCO	toluene	-5.27	-5.04		-9.36
hexan-1-ol	CCCCCCO	toluene	-6.17	-5.72		-10.46
heptan-1-ol	CCCCCCCO	toluene	-6.75	-6.50		-11.76
carbon disulfide	S=C=S	toluene	-3.53	-4.10		-5.82
sulfur hexafluoride	F[S](F)(F)(F)F	toluene	0.15	0.38	-1.27	-0.78
tetramethylstannane	C[Sn](C)(C)C	toluene	-3.77	-3.84		-6.29
benzene	c1ccccc1	toluene	-4.46	-4.41	-8.03	-7.87
toluene	Cc1ccccc1	toluene	-5.16	-5.18	-9.08	-9.10
ethylbenzene	CCc1ccccc1	toluene	-5.77	-5.93	-10.14	-10.25
o-xylene	Cc1ccccc1C	toluene	-6.12	-5.90		-10.25
p-xylene	Cc1ccc(C)cc1	toluene	-5.93	-5.89		-10.21
pyridine	c1ccncc1	toluene	-5.09	-5.07		-8.45
aniline	Nc1ccccc1	toluene	-6.78	-6.37		-10.84
benzonitrile	N#Cc1ccccc1	toluene	-7.21	-6.96		-11.16
2-methylaniline	Cc1ccccc1N	toluene	-7.56	-6.83		-11.79
pentanoic acid	CCCCC(O)=O	toluene	-5.89	-5.65		-10.49
chlorotrifluoromethane	FC(F)(F)Cl	toluene	-0.41	-0.19		-1.59
dichlorodifluoromethane	FC(F)(Cl)Cl	toluene	-1.38	-1.64		-3.73
helium	[He]	benzene	2.29	1.88	2.46	1.93
krypton	[Kr]	benzene	0.17	-0.11	-0.46	-0.80
xenon	[Xe]	benzene	-0.67	-1.10	-1.70	-2.35
hydrogen	[H][H]	benzene	1.57	1.38	1.52	1.13
deuterium	[H][H]	benzene	1.55	1.38		1.13
nitrogen	N#N	benzene	1.19	0.86	1.02	0.94
oxygen	O=O	benzene	0.85	0.58	0.41	0.07
nitrous oxide	[O-][N+]=N	benzene	-0.68	-0.88		-1.86

carbon monoxide	[C-]#[O+]	benzene	1.05	0.41	0.64	-0.19
carbon dioxide	O=C=O	benzene	-0.58	-0.62	-2.20	-1.94
sulfur hexafluoride	F[S](F)(F)(F)(F)F	benzene	0.19	0.23	-0.78	-0.82
methane	C	benzene	0.34	-0.19	-0.30	-1.00
ethane	CC	benzene	-0.84	-1.00	-2.00	-2.21
propane	CCC	benzene	-1.59	-1.71	-3.20	-3.32
butane	CCCC	benzene	-2.36	-2.37	-4.16	-4.34
2-methylpropane	CC(C)C	benzene	-2.10	-2.33		-4.28
pentane	CCCCC	benzene	-3.13	-3.12	-5.29	-5.51
hexane	CCCCCC	benzene	-3.84	-3.84	-6.37	-6.64
heptane	CCCCCCC	benzene	-4.56	-4.54	-7.41	-7.74
octane	CCCCCCCC	benzene	-5.19	-5.30	-8.48	-9.00
nonane	CCCCCCCCC	benzene	-5.88	-5.96	-9.48	-9.98
2-methylpentane	CCCC(C)C	benzene	-3.60	-3.69		-6.37
2,4-dimethylpentane	CC(C)CC(C)C	benzene	-4.01	-4.27		-7.28
cyclopropane	C1CC1	benzene	-2.13	-2.20		-3.85
cyclohexane	C1CCCCC1	benzene	-4.21	-4.20	-7.03	-7.03
ethylcyclohexane	CCC1CCCCC1	benzene	-5.34	-5.52		-9.09
ethene	C=C	benzene	-0.73	-1.04	-2.15	-2.25
propene	CC=C	benzene	-1.68	-1.83		-3.53
1-butene	CCC=C	benzene	-2.43	-2.50	-4.43	-4.54
cis-2-butene	C/C=C/C	benzene	-2.66	-2.63	-5.01	-4.83
trans-2-butene	C/C=C/C	benzene	-2.55	-2.59	-4.60	-4.72
2-methyl-2-propene	CC(C)=C	benzene	-2.39	-2.54		-4.67
1,3-butadiene	C=CC=C	benzene	-2.59	-2.64	-4.85	-4.82
tetrafluoromethane	FC(F)(F)F	benzene	1.19	1.01	0.54	0.45
difluoromethane	FCF	benzene	-0.85	-1.04		-2.34
trifluoromethane	FC(F)F	benzene	-0.24	-0.39		-1.33
1,1-difluoroethane	CC(F)F	benzene	-1.84	-2.13	-4.33	-4.27
2-chloro-2-methylpropane	CC(C)(C)Cl	benzene	-3.94	-4.12	-6.72	-7.34
1,2-dichloroethane	C1CCCl	benzene	-4.64	-4.46		-7.74
1,2-dichloropropane	CC(Cl)CCl	benzene	-4.90	-5.20		-8.92
1,3-dichloropropane	C1CCCl	benzene	-5.57	-5.14		-8.81
tetrachloroethene	ClC(Cl)=C(Cl)Cl	benzene	-6.48	-5.15		-8.85
dimethyl ether	COC	benzene	-2.26	-2.65	-5.04	-5.07
1,4-dioxane	C1COCCO1	benzene	-5.13	-5.25	-9.33	-9.35
ethanol	CCO	benzene	-3.22	-2.84	-7.08	-5.60
benzene	c1ccccc1	benzene	-4.56	-4.61	-8.09	-8.08
acetonitrile	CC#N	benzene	-3.87	-3.94	-7.46	-6.67
propionitrile	CCC#N	benzene	-4.49	-4.54	-8.70	-7.52
methyl acetate	COC(C)=O	benzene	-3.78	-4.34	-7.55	-8.02
ethyl acetate	CCOC(C)=O	benzene	-4.49	-4.77	-8.30	-8.66
butyl acetate	CCCCOC(C)=O	benzene	-5.80	-5.96	-10.30	-10.42
acetone	CC(C)=O	benzene	-3.82	-3.71	-7.19	-6.89
2-hexanone	CCCCC(C)=O	benzene	-5.76	-5.76	-10.08	-10.04
2-heptanone	CCCCCC(C)=O	benzene	-6.39	-6.41	-11.10	-11.03
cyclopentanone	O=C1CCCC1	benzene	-5.75	-5.58	-10.45	-9.79
nitromethane	C[N+](=O)[O-]	benzene	-4.37	-4.08	-8.37	-7.95
nitroethane	CC[N+](=O)[O-]	benzene	-4.94	-4.80	-9.15	-9.10
butylamine	CCCCN	benzene	-5.13	-4.12	-7.82	-7.48
sec-butylamine	CCC(C)N	benzene	-4.11	-3.57	-7.43	-6.85
tert-butylamine	CC(C)(C)N	benzene	-3.62	-3.54	-6.98	-7.05
cyclohexylamine	NC1CCCCC1	benzene	-4.85	-5.51	-9.75	-9.46
diethylamine	CCNCC	benzene	-4.01	-4.01	-7.60	-7.60
dipropylamine	CCNCCC	benzene	-5.09	-5.24	-9.51	-9.72
trimethylamine	CN(C)C	benzene	-2.76	-3.08		-5.78
triethylamine	CCN(CC)CC	benzene	-4.76	-4.83	-8.86	-8.74
benzaldehyde	O=Cc1ccccc1	benzene	-6.92	-6.62	-11.70	-11.28
pyridine	c1ccncc1	benzene	-5.27	-5.34	-9.61	-8.95
piperidine	C1CCNCC1	benzene	-5.03	-5.20		-8.91
phenol	Oc1ccccc1	benzene	-7.12	-6.09	-11.94	-10.72
hydrogen	[H][H]	ethyl acetate	1.46	1.03		0.43
nitrogen	N#N	ethyl acetate	1.04	1.09		0.81
nitric oxide	[N]=O	ethyl acetate	0.54	-0.26	-0.60	-1.84
sulfur dioxide	O=[S]=O	ethyl acetate	-3.22	-3.52	-7.10	-8.06
ethane	CC	ethyl acetate	-0.67	-0.56		-1.91
2-methylpropane	CC(C)C	ethyl acetate	-2.16	-1.91		-3.98
hexane	CCCCCC	ethyl acetate	-3.46	-3.48	-6.14	-6.45
heptane	CCCCCCC	ethyl acetate	-4.07	-4.12	-7.14	-7.41
octane	CCCCCCCC	ethyl acetate	-4.71	-4.67	-8.09	-8.17
nonane	CCCCCCCCC	ethyl acetate	-5.33	-5.40	-8.99	-9.35
2-methylpentane	CCCC(C)C	ethyl acetate	-3.29	-3.30	-5.70	-6.13
2,4-dimethylpentane	CC(C)CC(C)C	ethyl acetate	-3.69	-3.73		-6.73
2,3,4-trimethylpentane	CC(C)(C)C(C)C	ethyl acetate	-4.41	-4.15		-7.31
ethylcyclohexane	CCC1CCCCC1	ethyl acetate	-4.83	-5.00		-8.44
trans-but-2-ene	C/C=C/C	ethyl acetate	-2.77	-2.43		-4.93
pent-1-ene	CCCC=C	ethyl acetate	-2.96	-3.18		-6.14
2-methylprop-1-ene	CC(C)=C	ethyl acetate	-2.55	-2.24		-4.60
3-methylbut-1-ene	CC(C)C=C	ethyl acetate	-2.74	-3.00		-5.80
hept-1-ene	CCCCC=C	ethyl acetate	-4.07	-4.54		-8.21
buta-1,3-diene	C=CC=C	ethyl acetate	-2.84	-2.85		-5.78
2-methylbuta-1,3-diene	CC(=C)C=C	ethyl acetate	-3.29	-3.30		-6.39
hepta-1,6-diene	C=CCCC=C	ethyl acetate	-4.60	-4.99		-9.08

dichloromethane	CICCl	ethyl acetate	-4.04	-3.40		-6.47
tetrachloromethane	ClC(Cl)(Cl)Cl	ethyl acetate	-4.23	-4.75		-8.76
1,2-dichloroethane	CICCCl	ethyl acetate	-4.72	-4.47		-8.19
1-chloropropane	CCCCl	ethyl acetate	-3.68	-3.48		-6.73
1-chlorobutane	CCCCCl	ethyl acetate	-4.31	-4.08	-7.69	-7.65
2-chloro-2-methylpropane	CC(C)(C)Cl	ethyl acetate	-3.56	-3.69	-6.69	-7.05
2-bromo-2-methylpropane	CC(C)(C)Br	ethyl acetate	-4.05	-4.09	-7.34	-7.82
iodomethane	CI	ethyl acetate	-3.46	-3.12		-5.71
iodoethane	CCI	ethyl acetate	-4.04	-3.80		-6.78
1,1,2-trifluorotrichloroethane	FC(F)(Cl)C(F)(Cl)Cl	ethyl acetate	-3.40	-3.87		-7.63
1,2-difluorotetrachloroethane	FC(Cl)(Cl)C(F)(Cl)Cl	ethyl acetate	-4.62	-5.22		-9.72
tetrahydrofuran	C1CCOC1	ethyl acetate	-4.11	-4.02		-7.16
1,4-dioxane	C1COCCO1	ethyl acetate	-5.01	-4.82		-8.41
2-methylpropionaldehyde	CC(C)C=O	ethyl acetate	-4.05	-4.52		-8.45
propanone	CC(C)=O	ethyl acetate	-3.90	-3.66		-7.11
butanone	CCC(C)=O	ethyl acetate	-4.45	-4.41		-8.26
ethyl acetate	CCOC(C)=O	ethyl acetate	-4.50	-4.59	-8.40	-8.60
acetonitrile	CC#N	ethyl acetate	-4.19	-3.71		-5.84
diethylamine	CCNCC	ethyl acetate	-3.75	-4.18		-8.24
dimethylformamide	CN(C)C=O	ethyl acetate	-6.10	-6.08	-11.07	-11.36
methanol	CO	ethyl acetate	-3.68	-3.49	-7.62	-7.98
1-propanol	CCCO	ethyl acetate	-4.75	-4.86	-9.28	-10.17
1-butanol	CCCCO	ethyl acetate	-5.46	-5.43	-10.37	-11.02
propan-2-ol	CC(C)O	ethyl acetate	-4.13	-4.53		-9.54
dimethylsulfoxide	C[S](C)=O	ethyl acetate	-6.66	-7.03		-12.31
carbon disulfide	S=C=S	ethyl acetate	-3.12	-3.47		-4.40
tetramethylstannane	C[Sn](C)(C)C	ethyl acetate	-3.60	-3.98	-6.49	-6.38
benzene	c1ccccc1	ethyl acetate	-4.42	-4.41	-8.00	-7.90
toluene	Cc1ccccc1	ethyl acetate	-5.03	-4.93	-8.96	-8.66
chlorobenzene	Clc1ccccc1	ethyl acetate	-5.66	-5.85		-10.34
aniline	Nc1ccccc1	ethyl acetate	-7.49	-8.02	-14.17	-14.64
2-methylpyridine	Cc1ccccn1	ethyl acetate	-5.67	-6.44	-10.16	-10.79
2-furaldehyde	O=Cc1occc1	ethyl acetate	-6.30	-5.99		-11.05
hydrogen	[H][H]	methyl acetate	1.41	1.05	1.21	0.46
ozone	[O-][O+]=O	methyl acetate	-0.29	-1.06		-3.75
nitrogen	N#N	methyl acetate	0.92	1.03	0.68	0.80
nitrous oxide	[O-][N+]=N	methyl acetate	-1.09	-0.72		-1.92
carbon monoxide	[C-]#[O+]	methyl acetate	0.79	0.42	0.34	-0.41
carbon dioxide	O=C=O	methyl acetate	-1.13	-0.77		-2.57
ethane	CC	methyl acetate	-0.70	-0.55	-2.06	-1.77
pentane	CCCCC	methyl acetate	-2.68	-2.73	-5.20	-5.14
hexane	CCCCCC	methyl acetate	-3.30	-3.39	-5.78	-6.15
heptane	CCCCCCC	methyl acetate	-3.89	-4.03	-6.67	-7.11
nonane	CCCCCCCC	methyl acetate	-5.08	-5.31	-8.56	-9.04
2-methylpentane	CCCC(C)C	methyl acetate	-3.14	-3.20		-5.83
2,4-dimethylpentane	CC(C)CC(C)C	methyl acetate	-3.51	-3.64		-6.43
2,5-dimethylhexane	CC(C)CCC(C)C	methyl acetate	-4.10	-4.31		-7.46
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	methyl acetate	-4.22	-4.11		-7.14
ethylcyclohexane	CCC1CCCCC1	methyl acetate	-4.62	-4.91		-8.14
ethene	C=C	methyl acetate	-0.75	-1.10		-2.82
1-pentene	CCCC=C	methyl acetate	-2.88	-3.14		-5.95
1-hexene	CCCCC=C	methyl acetate	-3.51	-3.80		-6.93
acetylene	C#C	methyl acetate	-1.76	-1.62		-3.76
propyne	CC#C	methyl acetate	-2.51	-2.07		-4.31
1-butyne	CCC#C	methyl acetate	-3.03	-2.79		-5.45
but-1-en-3-yne	C=CC#C	methyl acetate	-3.19	-3.09		-6.09
dimethylether	COC	methyl acetate	-2.34	-2.42		-4.74
chloromethane	CCl	methyl acetate	-2.47	-2.01		-4.24
dichloromethane	CICCl	methyl acetate	-4.03	-3.39		-6.32
trans-1,2-dichloroethene	Cl/C=C\Cl	methyl acetate	-3.98	-4.30		-7.98
ethanol	CCO	methyl acetate	-4.10	-4.27	-8.33	-9.17
1-propanol	CCCO	methyl acetate	-4.89	-4.98		-10.30
isopropanol	CC(C)O	methyl acetate	-4.46	-4.61		-9.64
2-ethoxyethanol	CCOCCO	methyl acetate	-5.89	-5.92		-11.42
methyl acetate	COC(C)=O	methyl acetate	-4.14	-4.25	-7.72	-8.03
acetonitrile	CC#N	methyl acetate	-4.53	-3.91		-6.10
nitromethane	C[N+](=O)[O-]	methyl acetate	-5.13	-4.60		-9.23
nitroethane	CC[N+](=O)[O-]	methyl acetate	-5.46	-5.24		-10.11
acetone	CC(C)=O	methyl acetate	-4.02	-3.73		-7.13
ethyl oxirane	CCC1CO1	methyl acetate	-4.15	-3.91		-6.87
benzene	c1ccccc1	methyl acetate	-4.38	-4.38	-7.67	-7.72
water	O	methyl acetate	-3.98	-4.46		-10.64
hydrogen	[H][H]	butyl acetate	1.50	1.04		0.41
nitrous oxide	[O-][N+]=N	butyl acetate	-0.98	-0.39		-1.68
carbon monoxide	[C-]#[O+]	butyl acetate	0.87	0.58		-0.43
hexane	CCCCCC	butyl acetate	-3.59	-3.45		-6.64
heptane	CCCCCCC	butyl acetate	-4.23	-4.13		-7.68
octane	CCCCCCCC	butyl acetate	-4.85	-4.63		-8.33
nonane	CCCCCCCCC	butyl acetate	-5.49	-5.49		-9.78
2-methylpentane	CCCC(C)C	butyl acetate	-3.40	-3.28		-6.34
ethylcyclohexane	CCC1CCCCC1	butyl acetate	-4.99	-5.13		-8.96
1,6-heptadiene	C=CCCC=C	butyl acetate	-4.42	-5.00		-9.38
carbon tetrachloride	ClC(Cl)(Cl)Cl	butyl acetate	-4.26	-4.42		-8.30

butyl acetate	CCCCOC(C)=O	butyl acetate	-5.58	-5.66		-10.45
isobutanol	CC(C)CO	butyl acetate	-4.84	-4.99		-10.42
1-propanol	CCCO	butyl acetate	-4.65	-4.50		-9.71
1-pentanol	CCCCCO	butyl acetate	-6.28	-5.53		-11.12
3-methyl-1-butanol	CC(C)CCO	butyl acetate	-5.78	-5.68		-11.44
1-hexanol	CCCCCCO	butyl acetate	-6.83	-6.62		-13.01
cyclohexanol	OC1CCCCC1	butyl acetate	-7.07	-6.76		-12.90
1,3-dichloro-isopropanol	OC(CCl)CCl	butyl acetate	-7.58	-8.16		-15.45
benzene	c1ccccc1	butyl acetate	-3.87	-4.25		-7.87
toluene	Cc1ccccc1	butyl acetate	-5.50	-4.92		-8.91
<i>o</i> -xylene	Cc1ccccc1C	butyl acetate	-6.22	-5.50		-9.81
<i>m</i> -xylene	Cc1cccc(C)c1	butyl acetate	-6.06	-5.53		-9.86
<i>p</i> -xylene	Cc1ccc(C)cc1	butyl acetate	-6.10	-5.53		-9.86
n-octadecane	CCCCCCCCCCCCCCCC	butyl acetate	-11.94	-11.17		-18.42
carbon monoxide	[C-]#[O+]	propyl acetate	0.83	0.52		-0.42
hexane	CCCCCC	propyl acetate	-3.63	-3.48		-6.58
decane	CCCCCCCC	propyl acetate	-6.08	-6.10		-10.57
undecane	CCCCCCCCC	propyl acetate	-6.71	-6.65		-11.37
cyclohexane	C1CCCCC1	propyl acetate	-3.94	-3.90		-6.94
1-hexene	CCCC=C	propyl acetate	-3.78	-3.87		-7.33
1,7-octadiene	C=CCCCC=C	propyl acetate	-5.04	-5.60		-10.12
1-octyne	CCCCCCC#C	propyl acetate	-5.53	-5.55		-9.95
trichloromethane	ClC(Cl)Cl	propyl acetate	-4.65	-4.07		-7.57
isopropylbromide	CC(C)Br	propyl acetate	-3.97	-3.81		-7.48
benzene	c1ccccc1	propyl acetate	-4.48	-4.35		-7.92
ethylbenzene	CCc1ccccc1	propyl acetate	-5.63	-5.67		-9.95
<i>o</i> -xylene	Cc1ccccc1C	propyl acetate	-5.83	-5.46		-9.58
<i>p</i> -xylene	Cc1ccc(C)cc1	propyl acetate	-5.65	-5.48		-9.60
anisole	COc1ccccc1	propyl acetate	-6.57	-6.38		-11.26
tetrahydrofuran	C1CCOC1	propyl acetate	-4.14	-4.02		-7.28
acetone	CC(C)=O	propyl acetate	-3.82	-3.61		-7.13
ethyl acetate	CCOC(C)=O	propyl acetate	-4.43	-4.48		-8.49
acetonitrile	CC#N	propyl acetate	-4.25	-3.62		-5.74
ethanol	CCO	propyl acetate	-4.04	-4.04		-8.96
isopropanol	CC(C)O	propyl acetate	-4.30	-4.38		-9.44
anthracene	c1ccc2cc3ccccc3cc2c1	propyl acetate	-11.14	-10.77		-18.01
biphenyl	c1ccc(cc1)c2ccccc2	propyl acetate	-9.31	-9.12		-15.31
fluorobenzene	Fc1ccccc1	propyl acetate	-4.76	-4.76		-8.86
chlorobenzene	Clc1ccccc1	propyl acetate	-5.70	-5.90		-10.57
hydrogen	[H][H]	pentyl acetate	1.91	1.02		0.38
radon	[Rn]	pentyl acetate	-1.56	-0.80		-2.29
hexane	CCCCCC	pentyl acetate	-3.65	-3.45		-6.76
heptane	CCCCCCC	pentyl acetate	-4.31	-4.13		-7.80
octane	CCCCCCCC	pentyl acetate	-4.97	-4.63		-8.46
nonane	CCCCCCCCC	pentyl acetate	-5.61	-5.50		-9.90
decane	CCCCCCCCC	pentyl acetate	-6.20	-6.24		-11.06
cyclohexane	C1CCCCC1	pentyl acetate	-4.00	-3.93		-7.25
1-heptene	CCCCCC=C	pentyl acetate	-4.36	-4.53		-8.59
cyclohexene	C1CCC=CC1	pentyl acetate	-4.21	-4.12		-7.60
1-octyne	CCCCCCC#C	pentyl acetate	-5.50	-5.41		-9.90
trichloromethane	ClC(Cl)Cl	pentyl acetate	-4.60	-3.96		-7.62
1-chlorobutane	CCCCCl	pentyl acetate	-4.32	-4.25		-8.35
1,2-dichloropropane	CC(Cl)CCl	pentyl acetate	-4.89	-5.30		-9.95
isopropylbromide	CC(C)Br	pentyl acetate	-3.89	-3.89		-7.86
benzene	c1ccccc1	pentyl acetate	-4.44	-4.24		-7.96
ethylbenzene	CCc1ccccc1	pentyl acetate	-5.63	-5.67		-10.21
propylbenzene	CCCc1ccccc1	pentyl acetate	-6.20	-6.39		-11.33
<i>m</i> -xylene	Cc1cccc(C)c1	pentyl acetate	-5.76	-5.54		-10.01
tetrahydrofuran	C1CCOC1	pentyl acetate	-4.07	-3.92		-7.37
acetone	CC(C)=O	pentyl acetate	-3.62	-3.48		-7.19
ethyl acetate	CCOC(C)=O	pentyl acetate	-4.29	-4.40		-8.65
pentyl acetate	CCCCCOC(C)=O	pentyl acetate	-6.24	-6.30		-11.55
acetonitrile	CC#N	pentyl acetate	-3.98	-3.14		-5.12
ethanol	CCO	pentyl acetate	-3.89	-3.67		-8.45
isopropanol	CC(C)O	pentyl acetate	-4.07	-4.04		-8.98
nitromethane	C[N+](=O)=O	pentyl acetate	-4.69	-4.15		-8.82
fluorobenzene	Fc1ccccc1	pentyl acetate	-4.67	-4.61		-8.85
bromobenzene	Brc1ccccc1	pentyl acetate	-6.25	-6.27		-11.44
isobutyl acetate	CC(C)COC(C)=O	isobutyl acetate	-5.32	-5.64		-10.40
hydrogen	[H][H]	isobutyl acetate	1.49	0.96		0.34
carbon monoxide	[C-]#[O+]	isobutyl acetate	0.85	0.39		-0.76
ethyl butanoate	CCCC(=O)OCC	ethyl butanoate	-5.45	-5.84		-10.81
ethyl hexanoate	CCCCCC(=O)OCC	ethyl hexanoate	-6.61	-7.02		-12.83
hydrogen	[H][H]	2-methoxyethanol	1.84	1.38		0.55
heptane	CCCCCCC	2-methoxyethanol	-3.22	-3.45	-6.86	-6.80
octane	CCCCCCCC	2-methoxyethanol	-3.79	-4.00	-7.84	-7.66
nonane	CCCCCCCCC	2-methoxyethanol	-4.24	-4.85	-8.77	-9.07
decane	CCCCCCCCC	2-methoxyethanol	-4.73	-5.59	-9.70	-10.26
undecane	CCCCCCCCC	2-methoxyethanol	-5.16	-6.17	-10.66	-11.23
cyclohexane	C1CCCCC1	2-methoxyethanol	-3.18	-3.21	-6.36	-5.97
methylcyclopentane	CC1CCCC1	2-methoxyethanol	-2.99	-3.08		-5.75
methylcyclohexane	CC1CCCCC1	2-methoxyethanol	-3.47	-3.79	-6.79	-6.94
cyclooctane	C1CCCCCCC1	2-methoxyethanol	-4.55	-4.57		-8.17

cyclohexene	C1CCC=CC1	2-methoxyethanol	-3.49	-3.47		-6.42
1,7-octadiene	C=CCCCC=C	2-methoxyethanol	-4.09	-4.77		-8.84
4-vinyl-1-cyclohexene	C=CC1CCC=CC1	2-methoxyethanol	-4.43	-5.23		-9.36
ethanol	CCO	2-methoxyethanol	-4.84	-3.82		-8.85
2-methoxyethanol	COCCO	2-methoxyethanol	-5.96	-5.25	-10.80	-11.41
tetrahydrofuran	C1CCOC1	2-methoxyethanol	-3.92	-3.18		-5.72
1,4-dioxane	C1COCCO1	2-methoxyethanol	-4.95	-4.29		-7.68
nitromethane	C[N+](=O)[O-]	2-methoxyethanol	-4.97	-4.16		-8.11
benzene	c1ccccc1	2-methoxyethanol	-4.12	-3.83	-7.93	-7.22
toluene	Cc1ccccc1	2-methoxyethanol	-4.59	-4.54	-8.80	-8.35
ethylbenzene	CCc1ccccc1	2-methoxyethanol	-5.05	-5.23	-9.68	-9.38
<i>m</i> -xylene	Cc1ccc(C)c1	2-methoxyethanol	-5.10	-5.22	-9.66	-9.43
<i>p</i> -xylene	Cc1ccc(C)cc1	2-methoxyethanol	-5.07	-5.22	-9.63	-9.43
4-isopropyltoluene	CC(C)c1ccc(C)cc1	2-methoxyethanol	-5.75	-6.47		-11.38
fluorobenzene	Fc1ccccc1	2-methoxyethanol	-4.41	-4.27	-8.58	-8.05
chlorobenzene	Clc1ccccc1	2-methoxyethanol	-5.23	-5.36	-9.87	-9.68
bromobenzene	Brc1ccccc1	2-methoxyethanol	-5.74	-5.87	-10.64	-10.59
propanone	CC(C)=O	2-methoxyethanol	-3.79	-3.03		-5.83
methanol	CO	2-methoxyethanol	-4.25	-3.32		-8.01
acetonitrile	CC#N	2-methoxyethanol	-4.31	-3.63		-5.61
butyl acetate	CCCCOC(C)=O	2-methoxyethanol	-5.19	-5.11		-9.39
pyridine	c1ccncc1	2-methoxyethanol	-5.43	-5.30		-8.88
dichloromethane	ClCCl	2-methoxyethanol	-3.74	-2.98		-6.02
hydrogen	[H][H]	2-ethoxyethanol	1.70	1.28		0.30
2-methylpropane	CC(C)C	2-ethoxyethanol	-1.45	-1.43		-3.60
hexane	CCCCCC	2-ethoxyethanol	-3.03	-3.08		-6.23
heptane	CCCCCCC	2-ethoxyethanol	-3.60	-3.78		-7.35
octane	CCCCCCCC	2-ethoxyethanol	-4.16	-4.36		-8.25
nonane	CCCCCCCCC	2-ethoxyethanol	-4.73	-5.20		-9.64
decane	CCCCCCCCC	2-ethoxyethanol	-5.20	-5.95		-10.83
undecane	CCCCCCCCC	2-ethoxyethanol	-5.71	-6.55		-11.84
cyclohexane	C1CCCCC1	2-ethoxyethanol	-3.49	-3.48		-6.46
methylcyclopentane	CC1CCCC1	2-ethoxyethanol	-3.28	-3.36		-6.27
methylcyclohexane	CC1CCCCC1	2-ethoxyethanol	-3.79	-4.09		-7.47
cyclooctane	C1CCCCCCC1	2-ethoxyethanol	-4.92	-4.87		-8.70
cyclohexene	C1CCC=CC1	2-ethoxyethanol	-3.73	-3.68		-6.86
1,7-octadiene	C=CCCCC=C	2-ethoxyethanol	-4.37	-4.92		-9.12
4-vinyl-1-cyclohexene	C=CC1CCC=CC1	2-ethoxyethanol	-4.68	-5.41		-9.75
2-chloro-2-methylpropane	CC(C)(C)Cl	2-ethoxyethanol	-3.32	-3.27		-6.55
methanol	CO	2-ethoxyethanol	-4.34	-2.88		-7.20
ethanol	CCO	2-ethoxyethanol	-4.56	-3.57		-8.36
1-propanol	CCCO	2-ethoxyethanol	-5.33	-4.32		-9.60
ethyl acetate	CCOC(C)=O	2-ethoxyethanol	-4.14	-3.70		-7.10
propyl acetate	CCCOC(C)=O	2-ethoxyethanol	-4.71	-4.46		-8.41
ethyl propanoate	CCOC(=O)CC	2-ethoxyethanol	-4.58	-4.35		-8.18
2-ethoxyethanol	COCCO	2-ethoxyethanol	-6.23	-5.40		-11.14
toluene	Cc1ccccc1	2-ethoxyethanol	-4.70	-4.57		-8.46
ethylbenzene	CCc1ccccc1	2-ethoxyethanol	-5.19	-5.26		-9.52
<i>o</i> -xylene	Cc1ccccc1C	2-ethoxyethanol	-5.40	-5.24		-9.55
<i>m</i> -xylene	Cc1ccc(C)c1	2-ethoxyethanol	-5.24	-5.25		-9.55
<i>p</i> -xylene	Cc1ccc(C)cc1	2-ethoxyethanol	-5.19	-5.26		-9.55
4-isopropyltoluene	CC(C)c1ccc(C)cc1	2-ethoxyethanol	-5.98	-6.57		-11.60
fluorobenzene	Fc1ccccc1	2-ethoxyethanol	-4.38	-4.18		-8.04
chlorobenzene	Clc1ccccc1	2-ethoxyethanol	-5.42	-5.42		-9.92
1,2-dichlorobenzene	Clc1ccccc1Cl	2-ethoxyethanol	-6.61	-6.61		-11.88
bromobenzene	Brc1ccccc1	2-ethoxyethanol	-5.95	-5.90		-10.74
hexane	CCCCCC	2-butoxyethanol	-3.18	-3.03		-6.21
heptane	CCCCCCC	2-butoxyethanol	-3.86	-3.73		-7.33
octane	CCCCCCCC	2-butoxyethanol	-4.46	-4.31		-8.23
nonane	CCCCCCCCC	2-butoxyethanol	-5.06	-5.15		-9.62
decane	CCCCCCCCC	2-butoxyethanol	-5.59	-5.90		-10.81
cyclohexane	C1CCCCC1	2-butoxyethanol	-3.67	-3.43		-6.44
methylcyclopentane	CC1CCCC1	2-butoxyethanol	-3.46	-3.31		-6.25
methylcyclohexane	CC1CCCCC1	2-butoxyethanol	-4.01	-4.04		-7.45
cyclooctane	C1CCCCCCC1	2-butoxyethanol	-5.16	-4.82		-8.68
cyclohexene	C1CCC=CC1	2-butoxyethanol	-3.87	-3.63		-6.84
1,7-octadiene	C=CCCCC=C	2-butoxyethanol	-4.69	-4.86		-9.07
2-chloro-2-methylpropane	CC(C)(C)Cl	2-butoxyethanol	-3.30	-3.25		-6.58
toluene	Cc1ccccc1	2-butoxyethanol	-4.69	-4.43		-8.25
ethylbenzene	CCc1ccccc1	2-butoxyethanol	-5.22	-5.20		-9.46
<i>m</i> -xylene	Cc1ccc(C)c1	2-butoxyethanol	-5.31	-5.05		-9.18
<i>p</i> -xylene	Cc1ccc(C)cc1	2-butoxyethanol	-5.02	-5.05		-9.18
4-isopropyltoluene	CC(C)c1ccc(C)cc1	2-butoxyethanol	-6.33	-6.40		-11.33
naphthalene	c1ccc2ccccc2c1	2-butoxyethanol	-7.38	-7.16		-12.55
1,2-dichlorobenzene	Clc1ccccc1Cl	2-butoxyethanol	-6.47	-6.42		-11.57
bromobenzene	Brc1ccccc1	2-butoxyethanol	-5.80	-5.85		-10.72
2-butoxyethanol	CCCCOCCO	2-butoxyethanol	-7.11	-6.40		-12.78
hydrogen sulfide	S	diethylene glycol	-1.34	-0.99		-2.50
sulfur dioxide	O=[S]=O	diethylene glycol	-3.40	-3.44		-9.74
methane	C	diethylene glycol	1.26	0.88		-1.10
ethane	CC	diethylene glycol	0.47	0.25		-2.18
pentane	CCCCC	diethylene glycol	-0.86	-1.57		-5.08
hexane	CCCCCC	diethylene glycol	-1.47	-2.16		-6.00

heptane	CCCCCCC	diethylene glycol	-1.93	-2.73		-6.89
hexadecane	CCCCCCCCCCCCCCCC	diethylene glycol	-5.79	-8.96		-17.05
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	diethylene glycol	-1.75	-2.28		-6.11
methylcyclohexane	CC1CCCCC1	diethylene glycol	-2.38	-3.07		-7.02
ethylcyclohexane	CCC1CCCCC1	diethylene glycol	-2.89	-3.77		-8.16
1-pentene	CCCC=C	diethylene glycol	-1.23	-2.19		-6.16
1-heptene	CCCCC=C	diethylene glycol	-2.19	-3.37		-8.02
1-octene	CCCCC=C	diethylene glycol	-2.65	-3.92		-8.87
cyclohexene	C1CCC=CC1	diethylene glycol	-2.65	-2.91		-6.78
ethyne	C#C	diethylene glycol	-1.14	-0.84		-4.28
1-heptyne	CCCCC#C	diethylene glycol	-3.12	-3.54		-8.01
1-octyne	CCCCC#C	diethylene glycol	-3.68	-4.03		-8.72
dichloromethane	ClCCl	diethylene glycol	-3.35	-2.80		-7.12
trichloromethane	ClC(Cl)Cl	diethylene glycol	-3.84	-3.56		-8.37
1-chlorobutane	CCCCCl	diethylene glycol	-2.91	-3.57		-8.43
tert-butylchloride	CC(C)(C)Cl	diethylene glycol	-2.39	-3.04		-7.49
isopropylbromide	CC(C)Br	diethylene glycol	-2.74	-3.08		-7.73
benzene	c1ccccc1	diethylene glycol	-3.41	-3.55		-8.09
toluene	Cc1ccccc1	diethylene glycol	-3.86	-4.13		-9.00
ethylbenzene	CCc1ccccc1	diethylene glycol	-4.23	-4.70		-9.82
propylbenzene	CCCc1ccccc1	diethylene glycol	-4.55	-5.26		-10.66
isopropylbenzene	CC(C)c1ccccc1	diethylene glycol	-4.43	-5.23		-10.67
m-xylene	Cc1cccc(C)c1	diethylene glycol	-4.31	-4.67		-9.83
tetrahydrofuran	C1CCOC1	diethylene glycol	-3.53	-2.76		-6.30
1,4-dioxane	C1COCCO1	diethylene glycol	-4.49	-4.08		-8.64
methyl ethyl ketone	CCC(C)=O	diethylene glycol	-3.75	-3.22		-7.32
acetonitrile	CC#N	diethylene glycol	-4.12	-3.52		-6.76
nitromethane	C[N+](=O)=O	diethylene glycol	-4.56	-3.89		-8.86
fluorobenzene	Fc1ccccc1	diethylene glycol	-3.64	-4.09		-9.10
chlorobenzene	Clc1ccccc1	diethylene glycol	-4.63	-5.08		-10.55
bromobenzene	Br1ccccc1	diethylene glycol	-5.19	-5.60		-11.44
cyclopentane	C1CCCC1	diethylene glycol	-1.59	-1.85		-5.04
cycloheptane	C1CCCCC1	diethylene glycol	-2.88	-3.17		-7.14
cyclooctane	C1CCCCC1	diethylene glycol	-3.44	-3.85		-8.26
1-pentyne	CCCC#C	diethylene glycol	-2.34	-2.51		-6.55
ethanol	CCO	diethylene glycol	-4.56	-3.17		-8.97
carbon dioxide	O=C=O	triethylene glycol	-0.42	-0.03		-2.87
hydrogen sulfide	S	triethylene glycol	-0.92	-0.72		-1.56
methane	C	triethylene glycol	-0.65	1.29		0.45
ethane	CC	triethylene glycol	-1.38	0.58		-0.60
pentane	CCCCC	triethylene glycol	-3.40	-1.10		-3.30
hexane	CCCCC	triethylene glycol	3.00	-1.76		-4.34
octane	CCCCCCCC	triethylene glycol	-5.40	-2.99		-6.30
nonane	CCCCCCCCC	triethylene glycol	-5.88	-3.85		-7.72
undecane	CCCCCCCCCCC	triethylene glycol	-7.07	-5.16		-9.87
dodecane	CCCCCCCCCCCC	triethylene glycol	-7.71	-5.82		-10.93
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	triethylene glycol	-4.78	-2.01		-4.69
cyclopentane	C1CCCC1	triethylene glycol	-3.05	-1.48		-3.44
cyclohexane	C1CCCCC1	triethylene glycol	-3.50	-2.21		-4.62
cyclooctane	C1CCCCC1	triethylene glycol	-4.30	-3.57		-6.82
ethylcyclohexane	CCC1CCCCC1	triethylene glycol	-5.17	-3.50		-6.72
1-pentene	CCCC=C	triethylene glycol	-3.03	-1.74		-4.44
1-hexene	CCCCC=C	triethylene glycol	-3.48	-2.32		-5.33
1-heptene	CCCCC=C	triethylene glycol	-3.96	-2.94		-6.34
1-octene	CCCCC=C	triethylene glycol	-4.70	-3.63		-7.42
cis-2-hexene	CCC/C=C/C	triethylene glycol	-3.59	-2.25		-5.12
1,7-octadiene	C=CCCCC=C	triethylene glycol	-4.33	-4.02		-8.08
1-pentyne	CCCC#C	triethylene glycol	-2.25	-2.26		-5.34
1-hexyne	CCCCC#C	triethylene glycol	-3.24	-2.85		-6.23
1-octyne	CCCCC#C	triethylene glycol	-4.55	-3.97		-7.97
dichloromethane	ClCCl	triethylene glycol	-2.16	-2.18		-5.00
trichloromethane	ClC(Cl)Cl	triethylene glycol	-2.92	-2.94		-6.30
1-chlorobutane	CCCCCl	triethylene glycol	-2.86	-3.11		-6.71
tert-butylchloride	CC(C)(C)Cl	triethylene glycol	-3.58	-2.66		-6.02
benzene	c1ccccc1	triethylene glycol	-2.73	-2.87		-5.89
toluene	Cc1ccccc1	triethylene glycol	-3.14	-3.39		-6.64
ethylbenzene	CCc1ccccc1	triethylene glycol	-3.59	-4.11		-7.76
propylbenzene	CCCc1ccccc1	triethylene glycol	-4.16	-4.84		-8.92
isopropylbenzene	CC(C)c1ccccc1	triethylene glycol	-3.97	-4.69		-8.67
o-xylene	Cc1ccccc1C	triethylene glycol	-3.76	-4.03		-7.70
p-xylene	Cc1ccc(C)cc1	triethylene glycol	-3.60	-4.06		-7.71
tetrahydrofuran	C1CCOC1	triethylene glycol	-0.37	-2.38		-4.84
1,4-dioxane	C1COCCO1	triethylene glycol	0.51	-3.34		-6.31
acetone	CC(C)=O	triethylene glycol	0.47	-2.34		-5.32
butyl acetate	CCCCOC(C)=O	triethylene glycol	-1.68	-4.09		-8.02
acetonitrile	CC#N	triethylene glycol	-0.40	-2.97		-5.13
methanol	CO	triethylene glycol	0.54	-1.76		-5.47
ethanol	CCO	triethylene glycol	0.56	-2.10		-5.96
1-propanol	CCCO	triethylene glycol	-0.11	-2.67		-6.89
isopropanol	CC(C)O	triethylene glycol	0.27	-2.29		-6.29
fluorobenzene	Fc1ccccc1	triethylene glycol	-3.02	-3.47		-7.10
chlorobenzene	Clc1ccccc1	triethylene glycol	-3.76	-4.59		-8.84
bromobenzene	Br1ccccc1	triethylene glycol	-3.91	-5.15		-9.78

helium	[He]	pentane	1.72	1.84		1.77
neon	[Ne]	pentane	1.45	1.74		1.45
argon	[Ar]	pentane	0.30	0.31		-0.46
xenon	[Xe]	pentane	-0.98	-1.24	-2.62	-2.65
hydrogen	[H][H]	pentane	1.16	1.26		0.83
oxygen	O=O	pentane	0.49	0.73		0.15
nitrogen	N#N	pentane	0.72	0.84		0.71
nitrous oxide	[O-][N+][N]	pentane	-0.83	-0.72		-1.86
carbon monoxide	[C-]#[O+]	pentane	0.55	0.33		-0.39
ethane	CC	pentane	-1.01	-1.03		-2.59
n-butane	CCCC	pentane	-2.61	-2.53		-4.94
2-methylpropane	CC(C)C	pentane	-2.39	-2.41		-4.72
n-pentane	CCCCC	pentane	-3.40	-3.26		-6.08
n-hexane	CCCCCC	pentane	-4.05	-3.96		-7.18
n-heptane	CCCCCCC	pentane	-4.76	-4.67		-8.29
2,4-dimethylpentane	CC(C)CC(C)C	pentane	-4.31	-4.40		-7.76
n-octane	CCCCCCCC	pentane	-5.42	-5.39		-9.41
2,5-dimethylhexane	CC(C)CCC(C)C	pentane	-4.99	-5.11		-8.88
2,3,4-trimethylpentane	CC(C)(C)C(C)C	pentane	-5.03	-4.93		-8.55
n-nonane	CCCCCCCCC	pentane	-6.13	-6.08		-10.48
cyclohexane	C1CCCCC1	pentane	-4.23	-4.26		-7.52
ethylcyclohexane	CCC1CCCCC1	pentane	-5.39	-5.58		-9.54
ethene	C=C	pentane	-0.70	-0.98		-2.45
but-1-ene	CCC=C	pentane	-2.52	-2.47		-4.77
isobutene	CC(C)=C	pentane	-2.48	-2.40		-4.68
1-chlorobutane	CCCCCl	pentane	-4.08	-4.00		-7.27
1,4-dioxane	C1COCCO1	pentane	-4.04	-4.56		-8.38
furan	c1ccccc1	pentane	-3.28	-3.67		-6.94
butanone	CCC(C)=O	pentane	-3.42	-3.72		-6.94
butylamine	CCCCN	pentane	-3.70	-4.10		-7.62
nitromethane	C[N+](=[O-])=O	pentane	-2.69	-2.46		-5.14
water	O	pentane	-0.68	-0.85		-2.40
ethanol	CCO	pentane	-2.22	-2.33		-4.83
benzene	c1ccccc1	pentane	-4.01	-4.11		-7.33
toluene	Cc1ccccc1	pentane	-4.72	-4.75		-8.31
ethyl acetate	CCOC(C)=O	pentane	-3.54	-4.01		-7.53
propyl acetate	CCCOC(C)=O	pentane	-4.14	-4.66	-8.14	-8.53
butyl acetate	CCCCOC(C)=O	pentane	-4.98	-5.25	-9.58	-9.37
pentyl acetate	CCCCCOC(C)=O	pentane	-5.67	-5.88	-10.51	-10.33
methyl propanoate	CCC(=O)OC	pentane	-3.70	-4.10		-7.69
methyl pentanoate	CCCCC(=O)OC	pentane	-4.95	-5.34		-9.52
methyl hexanoate	CCCCCC(=O)OC	pentane	-5.67	-6.05		-10.61
helium	[He]	hexane	1.80	1.85	1.92	1.75
neon	[Ne]	hexane	1.58	1.72	1.30	1.41
argon	[Ar]	hexane	0.45	0.43	-0.65	-0.37
krypton	[Kr]	hexane	-0.16	-0.16	-1.13	-1.17
xenon	[Xe]	hexane	-0.93	-1.08	-2.56	-2.59
oxygen	O=O	hexane	0.58	0.77	-0.23	0.14
nitrogen	N#N	hexane	0.80	0.92	0.19	0.74
nitrous oxide	[O-][N+][N]	hexane	-0.74	-0.51		-1.62
nitric oxide	[N]=O	hexane	0.45	0.39	-0.53	-0.44
methane	C	hexane	0.03	-0.09	-0.54	-1.28
ethane	CC	hexane	-1.03	-1.00	-1.99	-2.72
propane	CCC	hexane	-1.80	-1.73	-3.37	-3.84
butane	CCCC	hexane	-2.55	-2.44	-4.90	-4.92
2-methylpropane	CC(C)C	hexane	-2.33	-2.35		-4.78
pentane	CCCCC	hexane	-3.33	-3.17	-6.39	-6.06
2,2-dimethylpropane	CC(C)(C)C	hexane	-2.77	-2.92	-5.15	-5.78
hexane	CCCCCC	hexane	-4.05	-3.87	-7.54	-7.14
2-methylpentane	CCCC(C)C	hexane	-3.85	-3.76		-6.96
2,2-dimethylbutane	CCC(C)(C)C	hexane	-3.64	-3.62	-6.64	-6.86
2,4-dimethylpentane	CC(C)CC(C)C	hexane	-4.38	-4.36	-7.81	-7.90
octane	CCCCCCC	hexane	-5.42	-5.35	-9.92	-9.54
2,5-dimethylhexane	CC(C)CCC(C)C	hexane	-4.97	-5.08		-9.01
nonane	CCCCCCCCC	hexane	-6.15	-6.02		-10.53
3,3-diethylpentane	CCC(CC)(CC)CC	hexane	-5.88	-5.70		-10.20
decane	CCCCCCCCC	hexane	-6.85	-6.73	-12.15	-11.63
dodecane	CCCCCCCCCCCC	hexane	-8.24	-8.15	-14.72	-13.92
cyclopropane	C1CC1	hexane	-1.98	-2.11		-4.15
cyclopentane	C1CCCC1	hexane	-3.70	-3.43	-6.76	-6.27
ethylcyclohexane	CCC1CCCCC1	hexane	-5.42	-5.41		-9.31
1-butene	CCC=C	hexane	-2.49	-2.46		-4.99
ethyne	C#C	hexane	-0.52	-0.89		-2.54
trichloromethane	ClC(Cl)Cl	hexane	-3.62	-3.59		-6.47
tetrachloromethane	ClC(Cl)(Cl)Cl	hexane	-4.13	-4.19	-7.74	-7.42
1-chloropropane	CCCCl	hexane	-3.37	-3.17		-6.01
1,2-dichloropropane	CC(Cl)CCl	hexane	-4.17	-4.44		-7.87
1,3-dichloropropane	C1CC1Cl	hexane	-4.43	-4.47		-7.93
1-chlorobutane	CCCCCl	hexane	-4.02	-3.88	-8.18	-7.11
2-chloro-2-methylpropane	CC(C)(C)Cl	hexane	-3.42	-3.59	-6.47	-6.72
1,4-dichlorobutane	C1CC1CCl	hexane	-4.95	-5.35		-9.34
1-chloropentane	CCCCCl	hexane	-4.78	-4.64		-8.32
bromoethane	CCBr	hexane	-3.14	-3.08		-6.07

2-bromo-2-methylpropane	CC(C)(C)Br	hexane	-3.75	-4.01		-7.43
dibromomethane	BrCBr	hexane	-3.98	-4.29		-8.03
iodoethane	CCl	hexane	-3.70	-3.91		-6.79
cfc12-cfc12	FC(Cl)(Cl)C(F)(Cl)Cl	hexane	-4.43	-4.90		-9.01
dimethyl ether	COC	hexane	-1.79	-2.16		-4.63
di-n-butylether	CCCCOCCCC	hexane	-5.91	-5.93		-10.30
ethyl t-butyl ether	CCOC(C)(C)C	hexane	-4.07	-4.07		-7.39
methyl t-pentyl ether	CCC(C)(C)OC	hexane	-4.47	-4.17		-7.59
tetrahydrofuran	C1CCOC1	hexane	-3.68	-4.02	-6.89	-7.57
1,4-dioxane	C1COCCO1	hexane	-4.07	-4.37	-7.45	-8.03
propanone	CC(C)=O	hexane	-2.68	-2.73		-5.34
butanone	CCC(C)=O	hexane	-3.40	-3.58		-6.71
hexan-2-one	CCCCC(C)=O	hexane	-4.68	-5.01		-8.95
heptan-2-one	CCCCC(C)=O	hexane	-5.36	-5.68		-10.03
ethyl acetate	CCOC(C)=O	hexane	-3.60	-3.82	-6.76	-7.19
propyl acetate	CCOC(C)=O	hexane	-4.03	-4.47	-7.99	-8.19
butyl acetate	CCCCOC(C)=O	hexane	-4.94	-5.09	-9.18	-9.15
pentyl acetate	CCCCCOC(C)=O	hexane	-5.57	-5.75	-10.16	-10.18
methyl propanoate	CCC(=O)OC	hexane	-3.65	-3.92		-7.36
methyl pentanoate	CCCCC(=O)OC	hexane	-4.93	-5.19		-9.29
methyl hexanoate	CCCCC(=O)OC	hexane	-5.65	-5.91		-10.42
acetonitrile	CC#N	hexane	-2.41	-2.70		-4.76
propionitrile	CCC#N	hexane	-3.04	-3.46	-5.76	-5.96
pentanonitrile	CCCC#N	hexane	-4.45	-4.78		-8.03
methylamine	CN	hexane	-1.64	-1.81		-3.87
ethylamine	CCN	hexane	-2.29	-2.50		-5.12
n-propylamine	CCCN	hexane	-3.08	-2.93		-5.94
isopropylamine	CC(C)N	hexane	-2.78	-2.85		-5.82
diethylamine	CCNCC	hexane	-3.57	-3.92		-7.83
triethylamine	CCN(CC)CC	hexane	-4.49	-4.86	-8.26	-9.16
nitromethane	C[N+](=[O-])=O	hexane	-2.76	-2.34	-5.40	-4.95
nitroethane	CC[N+](=[O-])=O	hexane	-3.42	-3.13	-6.60	-6.23
nitropropane	CCC[N+](=[O-])=O	hexane	-4.05	-4.00		-7.65
nitrobutane	CCCC[N+](=[O-])=O	hexane	-4.64	-4.66		-8.65
water	O	hexane	-0.74	-0.90		-2.71
methanol	CO	hexane	-1.57	-1.51	-3.61	-3.56
ethanol	CCO	hexane	-2.28	-2.23	-4.61	-4.75
propan-1-ol	CCCO	hexane	-3.02	-2.95		-5.91
propan-2-ol	CC(C)O	hexane	-2.76	-2.88		-5.82
butan-1-ol	CCCCO	hexane	-3.74	-3.65		-7.03
butan-2-ol	CCC(C)O	hexane	-3.56	-3.56		-6.91
2-methylpropan-1-ol	CC(C)CO	hexane	-3.58	-3.52		-6.83
pentan-1-ol	CCCCCO	hexane	-4.62	-4.40		-8.24
3-methylbutan-1-ol	CC(C)CCO	hexane	-4.05	-4.35		-8.19
hexan-1-ol	CCCCCO	hexane	-5.02	-5.10		-9.39
heptan-1-ol	CCCCCO	hexane	-5.59	-5.87		-10.65
dodecan-1-ol	CCCCCCCCCCCCO	hexane	-9.26	-9.38		-16.19
dimethyl sulfide	CSC	hexane	-2.97	-3.00		-5.32
sulfur hexafluoride	F[S](F)(F)(F)(F)F	hexane	-0.40	-0.38	-1.98	-1.85
tetramethylstannane	C[Sn](C)(C)C	hexane	-4.13	-4.15	-7.40	-7.11
benzene	c1ccccc1	hexane	-4.01	-4.15	-7.34	-7.64
toluene	Cc1ccccc1	hexane	-4.75	-4.76	-8.15	-8.54
ethylbenzene	CCc1ccccc1	hexane	-5.35	-5.48		-9.65
n-propylbenzene	CCCc1ccccc1	hexane	-5.55	-6.18		-10.73
1,2-dichlorobenzene	Clc1ccccc1Cl	hexane	-6.14	-6.01	-10.60	-10.29
1,3-dichlorobenzene	Clc1cccc(Cl)c1	hexane	-6.18	-6.20		-10.58
bromobenzene	Brc1ccccc1	hexane	-5.66	-5.67	-9.90	-9.96
benzaldehyde	O=Cc1ccccc1	hexane	-5.53	-5.54	-9.77	-9.62
acetophenone	CC(=O)c1ccccc1	hexane	-6.05	-6.27	-10.70	-10.77
nitrobenzene	[O-][N+](=O)c1ccccc1	hexane	-6.09	-5.68	-9.67	-10.11
pyridine	c1ccncc1	hexane	-4.19	-4.79	-7.67	-8.35
aniline	Nc1ccccc1	hexane	-5.43	-5.70	-11.19	-9.91
2-methylaniline	Cc1ccccc1N	hexane	-6.13	-6.15		-10.74
helium	[He]	heptane	1.89	1.85	1.85	1.72
neon	[Ne]	heptane	1.68	1.71	1.33	1.39
argon	[Ar]	heptane	0.52	0.54	-0.29	-0.30
krypton	[Kr]	heptane	-0.10	-0.07	-1.32	-1.18
xenon	[Xe]	heptane	-0.89	-0.93	-2.41	-2.52
oxygen	O=O	heptane	0.64	0.76		0.09
nitrogen	N#N	heptane	0.88	0.99		0.74
nitrous oxide	[O-][N+]=N	heptane	-0.65	-0.35		-1.49
carbon monoxide	[C-]#[O+]	heptane	0.75	0.61		-0.29
carbon dioxide	O=C=O	heptane	-0.41	0.09	-2.31	-1.11
iodine	I2	heptane	-4.66	-5.31		-8.74
methane	C	heptane	0.10	0.06	-0.91	-1.20
ethane	CC	heptane	-0.99	-0.88	-2.67	-2.68
propane	CCC	heptane	-1.77	-1.69	-4.09	-3.97
butane	CCCC	heptane	-2.53	-2.45		-5.16
2-methylpropane	CC(C)C	heptane	-2.31	-2.36		-5.01
pentane	CCCCC	heptane	-3.27	-3.18	-6.34	-6.30
hexane	CCCCCC	heptane	-3.96	-3.89	-7.54	-7.38
2-methylpentane	CCCC(C)C	heptane	-3.77	-3.78	-7.18	-7.20
heptane	CCCCCCC	heptane	-4.69	-4.61	-8.74	-8.53



2,4-dimethylpentane	CC(C)CC(C)C	heptane	-4.21	-4.37	-7.87	-8.13
octane	CCCCCCCC	heptane	-5.35	-5.37	-9.92	-9.78
2,5-dimethylhexane	CC(C)CCC(C)C	heptane	-4.87	-5.09		-9.24
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	heptane	-4.97	-4.94		-9.05
nonane	CCCCCCCCC	heptane	-6.07	-6.03	-11.09	-10.77
cyclopentane	C1CCCC1	heptane	-3.52	-3.44		-6.50
cyclohexane	C1CCCCC1	heptane	-4.19	-4.13	-7.72	-7.54
cycloheptane	C1CCCCC1	heptane	-5.04	-4.84	-9.04	-8.67
cyclooctane	C1CCCCCCC1	heptane	-5.83	-5.54	-10.20	-9.76
methylcyclohexane	CC1CCCCC1	heptane	-4.79	-4.70	-8.45	-8.39
ethylcyclohexane	CCC1CCCCC1	heptane	-5.37	-5.43		-9.55
cis-decalin	C1CC[C@@H]2CCCC[C@@H]2C1	heptane	-6.92	-6.95	-12.15	-11.61
ethene	C=C	heptane	-0.62	-0.82		-2.57
propene	CC=C	heptane	-1.74	-1.65		-3.90
1-butene	CCC=C	heptane	-2.48	-2.44		-5.15
isobutene	CC(C)=C	heptane	-2.44	-2.37		-5.04
1-pentene	CCCC=C	heptane	-3.15	-3.19		-6.31
3-methylbut-1-ene	CC(C)C=C	heptane	-2.96	-3.09		-6.15
hex-1-ene	CCCC=C	heptane	-3.83	-3.90		-7.41
hept-1-ene	CCCCC=C	heptane	-4.50	-4.62		-8.54
oct-1-ene	CCCCC=C	heptane	-5.17	-5.35		-9.72
1,3-butadiene	C=CC=C	heptane	-2.67	-2.42		-5.15
2-methylbuta-1,3-diene	CC(=C)C=C	heptane	-3.22	-3.11		-6.23
fluoroethane	CCF	heptane	-1.45	-1.16		-3.06
tetrafluoromethane	FC(F)(F)F	heptane	0.62	0.50	-0.38	-0.67
dichloromethane	ClCCl	heptane	-2.91	-2.81	-5.69	-5.56
trichloromethane	ClC(Cl)Cl	heptane	-3.62	-3.61	-6.74	-6.73
tetrachloromethane	ClC(Cl)(Cl)Cl	heptane	-4.09	-4.22	-7.46	-7.67
1,2-dichloroethane	ClCCCl	heptane	-3.70	-3.72	-6.69	-6.96
1-chloropropane	CCCCl	heptane	-3.29	-3.19		-6.26
2-chloro-2-methylpropane	CC(C)(C)Cl	heptane	-3.38	-3.52	-6.33	-6.72
bromoethane	CCBr	heptane	-3.04	-3.10		-6.30
iodomethane	Cl	heptane	-3.03	-3.23		-5.95
iodoethane	CCl	heptane	-3.68	-3.85		-6.86
difluorodichloromethane	FC(F)(Cl)Cl	heptane	-1.80	-1.94	-4.52	-4.65
trifluorochloromethane	FC(F)(F)Cl	heptane	-0.60	-0.72		-2.72
cfc12-cfc12	FC(Cl)(Cl)C(F)(Cl)Cl	heptane	-3.98	-4.76		-8.94
methyl t-butyl ether	COC(C)(C)C	heptane	-3.54	-3.51		-6.75
1,4-dioxane	C1COCCO1	heptane	-4.02	-4.30		-8.02
furan	c1ccoc1	heptane	-2.86	-3.54		-6.91
propanone	CC(C)=O	heptane	-2.55	-2.70		-5.44
pentan-2-one	CCCC(C)=O	heptane	-4.07	-4.21		-7.85
hexan-2-one	CCCCC(C)=O	heptane	-4.55	-4.99		-9.09
heptan-2-one	CCCCC(C)=O	heptane	-5.22	-5.64		-10.13
octan-2-one	CCCCC(C)=O	heptane	-5.68	-6.34		-11.18
3,3-dimethylbutan-2-one	CC(=O)C(C)(C)C	heptane	-4.30	-4.27		-7.85
cyclopentanone	O=C1CCCC1	heptane	-4.53	-4.56		-8.22
cyclohexanone	O=C1CCCCC1	heptane	-5.18	-5.25	-9.03	-9.31
ethyl acetate	CCOC(C)=O	heptane	-3.53	-3.75		-7.22
propyl acetate	CCOC(C)=O	heptane	-4.02	-4.43		-8.28
butyl acetate	CCCCOC(C)=O	heptane	-4.92	-5.05	-9.25	-9.24
pentyl acetate	CCCCCOC(C)=O	heptane	-5.48	-5.71	-10.64	-10.28
methyl propanoate	CCC(=O)OC	heptane	-3.63	-3.87		-7.43
methyl pentanoate	CCCCC(=O)OC	heptane	-4.91	-5.14	-9.19	-9.39
acetonitrile	CC#N	heptane	-2.28	-2.46	-4.20	-4.38
propionitrile	CCC#N	heptane	-2.86	-3.26	-5.83	-5.69
butyronitrile	CCCC#N	heptane	-3.68	-3.97	-6.83	-6.84
ethylamine	CCN	heptane	-2.09	-2.33		-4.97
n-propylamine	CCCN	heptane	-3.03	-2.75		-5.79
isopropylamine	CC(C)N	heptane	-2.62	-2.67	-5.47	-5.67
n-butylamine	CCCCN	heptane	-4.07	-3.58		-7.11
sec-butylamine	CCC(C)N	heptane	-3.34	-3.20	-6.67	-6.66
n-pentylamine	CCCCCN	heptane	-4.75	-4.41		-8.55
n-hexylamine	CCCCCN	heptane	-5.44	-4.88		-9.35
diethylamine	CCNCC	heptane	-3.44	-3.79	-6.79	-7.79
trimethylamine	CN(C)C	heptane	-2.44	-2.98		-6.26
triethylamine	CCN(CC)CC	heptane	-4.47	-4.70	-8.23	-9.05
cyclopentylamine	NC1CCCC1	heptane	-3.96	-4.93	-8.17	-9.05
nitroethane	CC[N+](=O)[O-]	heptane	-3.34	-3.01		-6.05
nitropropane	CCC[N+](=O)[O-]	heptane	-3.97	-3.89		-7.47
2-nitropropane	CC(C)[N+](=O)[O-]	heptane	-3.81	-3.78		-7.29
methanol	CO	heptane	-1.64	-1.48	-3.56	-3.71
ethanol	CCO	heptane	-2.24	-2.22	-4.45	-4.93
propan-1-ol	CCCO	heptane	-2.99	-2.94		-6.09
propan-2-ol	CC(C)O	heptane	-2.61	-2.87		-6.00
butan-1-ol	CCCCO	heptane	-3.75	-3.64	-6.66	-7.21
butan-2-ol	CCC(C)O	heptane	-3.26	-3.55		-7.09
2-methylpropan-2-ol	CC(C)(C)O	heptane	-3.01	-3.39		-7.02
pentan-1-ol	CCCCCO	heptane	-4.50	-4.39	-8.16	-8.42
hexan-1-ol	CCCCCO	heptane	-5.28	-5.09		-9.57
heptan-1-ol	CCCCCO	heptane	-5.59	-5.86		-10.82
2-ethoxyethanol	CCOCCO	heptane	-3.85	-4.56		-8.96

sulfur hexafluoride	F[S](F)(F)(F)(F)F	heptane	-0.31	-0.27	-1.98	-1.78
carbon disulfide	S=C=S	heptane	-3.33	-3.67		-4.71
benzene	c1ccccc1	heptane	-3.97	-4.18	-7.30	-7.91
toluene	Cc1ccccc1	heptane	-4.73	-4.79	-8.59	-8.80
o-xylene	Cc1ccccc1C	heptane	-5.51	-5.39		-9.70
n-propylbenzene	CCCc1ccccc1	heptane	-5.92	-6.21		-10.98
isopropylbenzene	CC(C)c1ccccc1	heptane	-5.72	-6.12		-10.83
1,2-dichlorobenzene	Clc1ccccc1Cl	heptane	-6.01	-6.04		-10.55
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	heptane	-5.81	-6.24	-10.61	-10.85
hexachlorobenzene	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	heptane	-10.24	-9.20		-15.39
bromobenzene	Brc1ccccc1	heptane	-5.72	-5.67		-10.16
fluorobenzene	Fc1ccccc1	heptane	-4.13	-4.14		-7.87
iodobenzene	Ic1ccccc1	heptane	-6.27	-6.28		-10.45
anisole	COc1ccccc1	heptane	-5.35	-5.35	-9.85	-9.50
benzaldehyde	O=Cc1ccccc1	heptane	-5.50	-5.55		-9.81
benzonitrile	N#Cc1ccccc1	heptane	-5.33	-5.95		-9.81
thiophene	s1ccccc1	heptane	-4.09	-4.15		-7.01
m-cresol	Cc1ccc(O)c1	heptane	-5.77	-5.72		-10.22
p-cresol	Cc1cc(O)cc1	heptane	-5.65	-5.73		-10.24
aniline	Nc1ccccc1	heptane	-5.38	-5.65	-9.74	-9.97
resorcinol	Oc1ccc(O)c1	heptane	-5.84	-6.37		-11.82
2-methylaniline	Cc1ccccc1N	heptane	-6.22	-6.11		-10.85
4-methylaniline	Cc1ccc(N)cc1	heptane	-6.14	-6.31		-11.05
helium	[He]	octane	1.98	1.84	1.93	1.70
neon	[Ne]	octane	1.73	1.69	1.66	1.36
argon	[Ar]	octane	0.60	0.62	-0.09	-0.26
krypton	[Kr]	octane	-0.03	0.01	-1.20	-1.19
xenon	[Xe]	octane	-0.85	-0.83	-2.43	-2.51
hydrogen	[H][H]	octane	1.35	1.45	0.97	0.97
oxygen	O=O	octane	0.70	0.72	0.03	-0.05
nitrogen	N#N	octane	0.97	1.03		0.63
nitrous oxide	[O-][N+][N]	octane	-0.60	-0.22		-1.41
carbon monoxide	[C-]#[O+]	octane	0.80	0.70	-0.27	-0.32
carbon dioxide	O=C=O	octane	-0.35	0.10	-1.94	-1.28
sulfur dioxide	O=[S]=O	octane	-1.01	-2.11		-4.49
ethane	CC	octane	-0.96	-0.76		-2.63
propane	CCC	octane	-1.75	-1.57		-3.92
butane	CCCC	octane	-2.50	-2.36		-5.16
hexane	CCCCCC	octane	-3.90	-3.90		-7.59
heptane	CCCCCCC	octane	-4.60	-4.62		-8.74
2,4-dimethylpentane	CC(C)CC(C)C	octane	-4.13	-4.38		-8.34
octane	CCCCCCCC	octane	-5.33	-5.38	-9.92	-10.00
2,5-dimethylhexane	CC(C)CCCC(C)C	octane	-4.83	-5.09		-9.45
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	octane	-4.46	-4.85	-8.39	-9.16
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	octane	-4.91	-4.95		-9.25
cyclohexane	C1CCCCC1	octane	-4.16	-4.15		-7.77
ethylcyclohexane	CCC1CCCCC1	octane	-5.37	-5.44		-9.77
propene	CC=C	octane	-1.71	-1.54		-3.86
1-butene	CCC=C	octane	-2.45	-2.32		-5.10
isobutene	CC(C)=C	octane	-2.41	-2.26		-5.00
1-pentene	CCCC=C	octane	-3.10	-3.11		-6.33
3-methylbut-1-ene	CC(C)C=C	octane	-2.92	-3.00		-6.15
2-methylbuta-1,3-diene	CC(=C)C=C	octane	-3.18	-3.00		-6.19
tetrafluoromethane	FC(F)(F)F	octane	0.72	0.56	-0.02	-0.62
dichloromethane	ClCCl	octane	-2.86	-2.75		-5.61
trichloromethane	ClC(Cl)Cl	octane	-3.52	-3.57		-6.82
tetrachloromethane	ClC(Cl)(Cl)Cl	octane	-3.98	-4.16		-7.74
1-chloropropane	CCCCl	octane	-3.22	-3.22		-6.49
2-chloro-2-methylpropane	CC(C)(C)Cl	octane	-3.36	-3.52	-6.33	-6.89
bromoethane	CCBr	octane	-2.99	-3.11		-6.49
iodomethane	CI	octane	-2.99	-3.17		-6.00
difluorodichloromethane	FC(F)(Cl)Cl	octane	-1.76	-1.88		-4.61
diethyl ether	CCOCC	octane	-3.05	-3.33	-6.19	-6.68
diisopropyl ether	CC(C)OC(C)C	octane	-3.84	-4.28	-7.44	-8.10
di-n-butylether	CCCCOCCCC	octane	-5.78	-5.93		-10.69
tetrahydrofuran	C1CCOC1	octane	-3.66	-3.82		-7.43
furan	c1ccccc1	octane	-2.84	-3.53		-7.04
propanal	CCC=O	octane	-2.54	-2.80		-5.77
butanal	CCCC=O	octane	-3.23	-3.51		-6.88
pentanal	CCCCC=O	octane	-3.97	-4.32		-8.21
hexanal	CCCCCC=O	octane	-4.76	-5.02		-9.26
propanone	CC(C)=O	octane	-2.52	-2.68		-5.57
butanone	CCC(C)=O	octane	-3.23	-3.53		-6.95
pentan-2-one	CCCC(C)=O	octane	-3.87	-4.20		-7.98
4-methylpentan-2-one	CC(C)CC(C)=O	octane	-4.34	-4.86		-9.09
heptan-2-one	CCCCCC(C)=O	octane	-5.25	-5.59		-10.19
3,3-dimethylbutan-2-one	CC(=O)C(C)(C)C	octane	-4.21	-4.22		-7.90
methyl acetate	COC(C)=O	octane	-2.88	-3.08		-6.30
ethyl acetate	CCOC(C)=O	octane	-3.40	-3.70	-6.96	-7.27
propyl acetate	CCCOC(C)=O	octane	-4.02	-4.37		-8.33
butyl acetate	CCCCOC(C)=O	octane	-4.90	-4.99		-9.29
methyl propanoate	CCC(=O)OC	octane	-3.57	-3.82	-7.01	-7.48
ethyl propanoate	CCOC(=O)CC	octane	-4.11	-4.42		-8.44

ethyl butanoate	CCCC(=O)OCC	octane	-4.69	-5.07		-9.47
methyl pentanoate	CCCCC(=O)OC	octane	-4.85	-5.09		-9.44
methyl hexanoate	CCCCC(=O)OC	octane	-5.55	-5.81	-10.47	-10.58
propionitrile	CCC#N	octane	-2.84	-3.14		-5.58
ethylamine	CCN	octane	-2.05	-2.18		-4.84
n-propylamine	CCCN	octane	-3.00	-2.59		-5.65
n-butylamine	CCCCN	octane	-3.44	-3.42		-6.97
nitromethane	C[N+](=O)=O	octane	-2.62	-2.19		-4.80
nitroethane	CC[N+](=O)=O	octane	-3.37	-2.95		-6.04
nitropropane	CCC[N+](=O)=O	octane	-3.95	-3.84		-7.50
water	O	octane	-0.68	-0.97	-2.49	-3.30
methanol	CO	octane	-1.45	-1.33	-3.66	-3.57
ethanol	CCO	octane	-2.18	-2.13	-4.66	-4.92
propan-1-ol	CCCO	octane	-2.91	-2.92		-6.22
butan-1-ol	CCCCO	octane	-3.62	-3.62		-7.34
2-methylpropan-1-ol	CC(C)CO	octane	-3.33	-3.49		-7.14
butan-2-ol	CCC(C)O	octane	-3.26	-3.53		-7.22
pentan-1-ol	CCCCCO	octane	-4.27	-4.36		-8.56
3-methylbutan-1-ol	CC(C)CCO	octane	-3.98	-4.32		-8.50
2-methyl-1-pentanol	CCCC(C)CO	octane	-4.89	-4.91		-9.43
2-methyl-2-pentanol	CCCC(C)(C)O	octane	-4.59	-4.68		-9.27
3-methyl-2-pentanol	CCC(C)(C)O	octane	-4.87	-4.67		-9.10
4-methyl-1-pentanol	CC(C)CCO	octane	-4.84	-4.95		-9.43
2-methyl-3-pentanol	CCC(O)C(C)C	octane	-4.72	-4.65		-9.08
4-methyl-2-pentanol	CC(C)CC(C)O	octane	-4.63	-4.77		-9.29
2,3-dimethyl-2-butanol	CC(C)(C)(C)O	octane	-4.60	-4.54		-9.08
3-methyl-3-hexanol	CCCC(C)(O)CC	octane	-5.40	-5.35		-10.36
3-methyl-2-hexanol	CCCC(C)(C)O	octane	-5.31	-5.36		-10.21
2-methyl-2-hexanol	CCCC(C)(C)O	octane	-5.29	-5.26		-10.25
5-methyl-2-hexanol	CC(C)CCC(C)O	octane	-5.33	-5.41		-10.26
4,4-dimethyl-2-pentanol	CC(O)CC(C)(C)C	octane	-5.41	-5.01		-9.80
2,3-dimethyl-3-pentanol	CCC(C)(O)C(C)C	octane	-5.40	-5.13		-10.03
carbon disulfide	S=C=S	octane	-3.29	-3.50		-4.46
benzene	c1ccccc1	octane	-3.96	-4.11		-7.95
m-cresol	Cc1cccc(O)c1	octane	-5.79	-5.70		-10.37
p-cresol	Cc1ccc(O)cc1	octane	-5.63	-5.72		-10.38
aniline	Nc1ccccc1	octane	-4.84	-5.51		-9.85
4-methylaniline	Cc1ccc(N)cc1	octane	-6.29	-6.25		-11.08
helium	[He]	nonane	2.04	1.83	2.32	1.68
neon	[Ne]	nonane	1.82	1.68	1.50	1.34
krypton	[Kr]	nonane	0.02	0.08	-1.11	-1.19
xenon	[Xe]	nonane	-0.82	-0.77	-2.38	-2.53
hydrogen	[H][H]	nonane	1.39	1.48		1.00
oxygen	O=O	nonane	0.73	0.70		-0.16
methane	C	nonane	0.20	0.16		-1.11
propane	CCC	nonane	-1.71	-1.47		-3.85
n-pentane	CCCCC	nonane	-3.18	-3.06		-6.38
n-hexane	CCCCCC	nonane	-3.86	-3.83		-7.60
2-methylpentane	CCCC(C)C	nonane	-3.67	-3.71		-7.40
2,4-dimethylpentane	CC(C)CC(C)C	nonane	-4.09	-4.35		-8.42
n-octane	CCCCCCC	nonane	-5.21	-5.35		-10.06
2,3,4-trimethylpentane	CC(C)(C)(C)C(C)C	nonane	-4.87	-4.93		-9.35
n-nonane	CCCCCCCCC	nonane	-5.98	-6.05		-11.10
cyclohexane	C1CCCCC1	nonane	-4.13	-4.17		-7.94
ethene	C=C	nonane	-0.58	-0.61		-2.47
propene	CC=C	nonane	-1.69	-1.44		-3.80
isobutene	CC(C)=C	nonane	-2.39	-2.16		-4.94
sulfur hexafluoride	F[S](F)(F)(F)F	nonane	-0.14	-0.10		-1.62
methyl ethyl ketone	CCC(C)=O	nonane	-3.28	-3.50		-7.02
2-pentanone	CCCC(C)=O	nonane	-3.96	-4.21		-8.14
2-hexanone	CCCCC(C)=O	nonane	-4.58	-4.88		-9.16
2-heptanone	CCCCC(C)=O	nonane	-5.27	-5.53		-10.17
methyl acetate	COC(C)=O	nonane	-2.83	-2.90		-6.06
propyl acetate	CCCOC(C)=O	nonane	-4.01	-4.31		-8.32
pentyl acetate	CCCCCOC(C)=O	nonane	-5.39	-5.59		-10.32
methyl propanoate	CCC(=O)OC	nonane	-3.51	-3.72		-7.40
methyl pentanoate	CCCCC(=O)OC	nonane	-4.85	-5.03		-9.44
helium	[He]	decane	2.08	1.82	1.64	1.66
neon	[Ne]	decane	1.86	1.67	1.56	1.32
argon	[Ar]	decane	0.69	0.69	-0.39	-0.21
krypton	[Kr]	decane	0.06	0.13	-1.16	-1.19
xenon	[Xe]	decane	-0.78	-0.71	-2.35	-2.54
hydrogen	[H][H]	decane	1.49	1.49		1.01
oxygen	O=O	decane	0.77	0.68	-0.06	-0.24
nitrogen	N#N	decane	1.09	1.09	-0.07	0.50
carbon dioxide	O=C=O	decane	0.27	0.16	-1.65	-1.47
methane	C	decane	0.24	0.19	-1.03	-1.06
ethane	CC	decane	-0.89	-0.59	-1.86	-2.52
2-methylpropane	CC(C)C	decane	-2.23	-2.08		-4.89
pentane	CCCCC	decane	-3.12	-2.96		-6.30
hexane	CCCCCC	decane	-3.81	-3.74	-7.53	-7.53
2-methylpentane	CCCC(C)C	decane	-3.62	-3.62	-7.11	-7.34
2,2-dimethylbutane	CCC(C)(C)C	decane	-3.38	-3.24	-6.56	-6.75

heptane	CCCCCCC	decane	-4.50	-4.51		-8.77
2,4-dimethylpentane	CC(C)CC(C)C	decane	-4.05	-4.26		-8.35
2,5-dimethylhexane	CC(C)CCC(C)C	decane	-4.73	-5.04		-9.59
nonane	CCCCCCCCC	decane	-5.93	-6.03		-11.21
decane	CCCCCCCCC	decane	-6.60	-6.78	-12.28	-12.38
cyclopentane	C1CCCC1	decane	-3.46	-3.42		-6.89
methylcyclopentane	CC1CCCC1	decane	-3.93	-4.09		-7.92
cyclohexane	C1CCCCC1	decane	-4.08	-4.16		-8.05
ethylcyclohexane	CCC1CCCCC1	decane	-5.27	-5.48		-10.09
propene	CC=C	decane	-1.68	-1.36		-3.75
1-butene	CCC=C	decane	-2.42	-2.15		-4.99
isobutene	CC(C)=C	decane	-2.36	-2.08		-4.88
tetrafluoromethane	FC(F)(F)F	decane	0.86	0.65		-0.51
trichloroethene	ClC=C(Cl)Cl	decane	-3.84	-3.89		-7.60
methyl t-butyl ether	COC(C)(C)C	decane	-3.48	-3.29		-6.71
1,4-dioxane	C1COCCO1	decane	-3.97	-4.22		-8.25
furan	c1ccoc1	decane	-2.76	-3.31		-6.82
propanone	CC(C)=O	decane	-2.47	-2.50		-5.44
butanone	CCC(C)=O	decane	-3.27	-3.42		-6.95
hexan-2-one	CCCCC(C)=O	decane	-4.61	-4.85		-9.19
heptan-2-one	CCCCCC(C)=O	decane	-5.18	-5.46		-10.15
3,3-dimethylbutan-2-one	CC(=O)C(C)(C)C	decane	-4.15	-4.09		-7.86
ethyl acetate	CCOC(C)=O	decane	-3.28	-3.44		-6.96
propyl acetate	CCCOC(C)=O	decane	-3.96	-4.20		-8.19
butyl acetate	CCCCOC(C)=O	decane	-4.75	-4.86		-9.25
pentyl acetate	CCCCCOC(C)=O	decane	-5.37	-5.52		-10.29
methyl propanoate	CCC(=O)OC	decane	-3.49	-3.55		-7.14
methyl pentanoate	CCCCC(=O)OC	decane	-4.75	-4.95		-9.38
methyl hexanoate	CCCCCC(=O)OC	decane	-5.48	-5.69	-10.44	-10.54
ethylamine	CCN	decane	-1.93	-1.90		-4.52
n-propylamine	CCCN	decane	-2.97	-2.32		-5.36
n-butylamine	CCCCN	decane	-3.40	-3.14		-6.66
nitromethane	C[N+](=O)[O-]	decane	-2.62	-2.17		-4.98
water	O	decane	-0.48	-1.01	-1.65	-3.53
methanol	CO	decane	-1.41	-1.04	-3.78	-3.24
ethanol	CCO	decane	-2.16	-1.86		-4.64
propan-1-ol	CCCO	decane	-2.76	-2.68		-5.98
butan-1-ol	CCCCO	decane	-3.77	-3.39		-7.13
pentan-1-ol	CCCCCO	decane	-4.16	-4.22		-8.50
2-methyl-2-butanol	CCC(C)(C)O	decane	-3.99	-3.79	-6.76	-8.03
2-methyl-1-pentanol	CCCC(C)CO	decane	-4.82	-4.80		-9.45
2-methyl-2-pentanol	CCCC(C)(C)O	decane	-4.54	-4.50		-9.16
3-methyl-2-pentanol	CCC(C)C(C)O	decane	-4.81	-4.56		-9.13
4-methyl-1-pentanol	CC(C)CCCCO	decane	-4.78	-4.85		-9.47
2-methyl-3-pentanol	CCC(O)C(C)C	decane	-4.67	-4.53		-9.10
4-methyl-2-pentanol	CC(C)CC(C)O	decane	-4.56	-4.64		-9.30
2,3-dimethyl-2-butanol	CC(C)C(C)(C)O	decane	-4.55	-4.40		-9.03
3,3-dimethyl-1-butanol	CC(C)(C)CCO	decane	-4.72	-4.47		-9.16
3-methyl-3-hexanol	CCCC(C)(O)CC	decane	-5.34	-5.22		-10.35
2-methyl-3-hexanol	CCCC(O)C(C)C	decane	-5.46	-5.26		-10.27
3-methyl-2-hexanol	CCCC(C)C(C)O	decane	-5.27	-5.28		-10.31
2-methyl-2-hexanol	CCCCC(C)(C)O	decane	-5.22	-5.10		-10.17
5-methyl-2-hexanol	CC(C)CCCCO	decane	-5.22	-5.33		-10.36
3-ethyl-3-pentanol	CCC(O)(CC)CC	decane	-5.34	-5.11		-10.21
2,3-dimethyl-3-pentanol	CCC(C)(O)C(C)C	decane	-5.34	-5.00		-10.03
2,2-dimethyl-3-pentanol	CCC(O)C(C)(C)C	decane	-4.85	-4.90		-9.82
sulfur hexafluoride	F[S](F)(F)(F)(F)F	decane	-0.06	-0.09	-1.89	-1.64
benzene	c1ccccc1	decane	-3.98	-3.95		-7.86
toluene	Cc1ccccc1	decane	-4.67	-4.65		-8.94
ethylbenzene	CCc1ccccc1	decane	-5.23	-5.41		-10.10
n-propylbenzene	CCCc1ccccc1	decane	-5.23	-6.16		-11.29
fluorobenzene	Fc1ccccc1	decane	-3.48	-3.87		-7.75
chlorobenzene	Clc1ccccc1	decane	-4.93	-5.20		-9.77
bromobenzene	Brc1ccccc1	decane	-5.43	-5.67		-10.53
2-furaldehyde	O=Cc1occc1	decane	-4.51	-4.32		-8.38
5-methylfurfural	Cc1oc(C=O)cc1	decane	-5.29	-5.33		-9.86
2-methylaniline	Cc1ccccc1N	decane	-6.64	-5.70		-10.42
4-methylaniline	Cc1ccc(N)cc1	decane	-6.48	-5.99		-10.78
neon	[Ne]	undecane	1.90	1.67		1.31
argon	[Ar]	undecane	0.72	0.70		-0.20
krypton	[Kr]	undecane	0.08	0.17		-1.17
hydrogen	[H][H]	undecane	1.50	1.50		1.02
nitrogen	N#N	undecane	1.12	1.10		0.49
methane	C	undecane	0.27	0.21		-1.01
hexane	CCCCC	undecane	-3.96	-3.68		-7.47
decane	CCCCCCCCC	undecane	-6.77	-6.72		-12.33
undecane	CCCCCCCCCCC	undecane	-7.48	-7.40	-13.46	-13.44
dodecane	CCCCCCCCCCCC	undecane	-8.19	-8.12		-14.58
tetrafluoromethane	FC(F)(F)F	undecane	0.93	0.67		-0.46
chloroform	ClC(Cl)Cl	undecane	-3.45	-3.34		-6.69
carbon tetrachloride	ClC(Cl)(Cl)Cl	undecane	-3.66	-3.94		-7.65
1,2-dichloroethane	ClCCCl	undecane	-3.52	-3.70		-7.38
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	undecane	-3.59	-4.51		-8.55

1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	undecane	-5.07	-5.57		-10.13
1,2- <i>trans</i> -dichloroethene	ClC=C(Cl)	undecane	-3.44	-3.21		-6.61
trichloroethene	ClC=C(Cl)Cl	undecane	-3.74	-3.85		-7.59
bromoform	BrC(Br)Br	undecane	-4.82	-5.29		-9.97
bis(2-chloroethyl)ether	ClCCOCCl	undecane	-5.77	-5.76		-10.23
acrolein	C=CC=O	undecane	-2.76	-2.31		-5.23
acrylonitrile	C=CC#N	undecane	-1.95	-2.78		-5.12
sulfur hexafluoride	F[S](F)(F)(F)(F)F	undecane	0.01	-0.08		-1.64
benzene	c1ccccc1	undecane	-3.86	-3.88		-7.80
toluene	Cc1ccccc1	undecane	-4.62	-4.56		-8.82
ethylbenzene	CCc1ccccc1	undecane	-5.25	-5.32		-9.98
nitrobenzene	[O-][N+](=O)c1ccccc1	undecane	-6.08	-5.44		-10.07
furfuryl acetate	CC(=O)OCCc1occc1	undecane	-5.92	-5.95		-10.74
helium	[He]	dodecane	2.14	1.79	1.72	1.62
argon	[Ar]	dodecane	0.75	0.71	-0.15	-0.19
krypton	[Kr]	dodecane	0.12	0.21	-1.02	-1.16
xenon	[Xe]	dodecane	-0.72	-0.65	-2.28	-2.56
hydrogen	[H][H]	dodecane	1.51	1.50		1.02
oxygen	O=O	dodecane	0.83	0.67		-0.27
nitrogen	N#N	dodecane	1.16	1.10		0.46
carbon monoxide	[C-]#[O+]	dodecane	1.06	0.79		-0.33
carbon dioxide	O=C=O	dodecane	-0.26	0.29	-1.43	-1.21
ethane	CC	dodecane	-0.79	-0.56		-2.43
propane	CCC	dodecane	-1.51	-1.26	-3.65	-3.69
butane	CCCC	dodecane	-2.26	-2.05		-4.94
pentane	CCCCC	dodecane	-3.08	-2.84		-6.19
2-methylbutane	CCC(C)C	dodecane	-2.88	-2.73		-6.01
2,2-dimethylpropane	CC(C)(C)C	dodecane	-2.46	-2.32		-5.33
hexane	CCCCCC	dodecane	-3.72	-3.61	-7.51	-7.42
2-methylpentane	CCCC(C)C	dodecane	-3.51	-3.50		-7.23
heptane	CCCCCCC	dodecane	-4.42	-4.39	-8.72	-8.66
2,4-dimethylpentane	CC(C)CC(C)C	dodecane	-3.94	-4.13	-7.72	-8.24
octane	CCCCCCCC	dodecane	-5.12	-5.09	-9.90	-9.80
2,5-dimethylhexane	CC(C)CCC(C)C	dodecane	-4.62	-4.91		-9.48
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	dodecane	-4.73	-4.71		-9.17
nonane	CCCCCCCCC	dodecane	-5.80	-5.89		-11.06
dodecane	CCCCCCCCCCCC	dodecane	-7.97	-8.04	-14.75	-14.47
cyclopentane	C1CCCC1	dodecane	-3.37	-3.30		-6.79
cyclohexane	C1CCCCC1	dodecane	-4.02	-4.04		-7.95
ethene	C=C	dodecane	-0.50	-0.47		-2.40
1-pentene	CCCC=C	dodecane	-2.92	-2.81		-6.12
2-methyl-1,3-butadiene	CC(=C)C=C	dodecane	-3.00	-2.73		-6.04
<i>cis</i> -1,3-pentadiene	C\C=C/C=C	dodecane	-3.18	-2.80		-6.12
<i>trans</i> -1,3-pentadiene	C/C=C/C=C	dodecane	-3.15	-2.83		-6.17
carbon tetrafluoride	FC(F)(F)F	dodecane	0.98	0.69		-0.41
bis(2,2,2-trifluoroethyl)ether	FC(F)(F)COCC(F)(F)F	dodecane	-2.01	-2.51		-6.68
furan	c1ccoc1	dodecane	-2.71	-3.14		-6.59
acetone	CC(C)=O	dodecane	-2.47	-2.27		-5.11
2,4-pentanedione	CC(=O)CC(C)=O	dodecane	-4.62	-4.60		-8.75
2,4-hexanedione	CCC(=O)CC(C)=O	dodecane	-5.29	-5.20		-9.70
2,4-heptanedione	CCCC(=O)CC(C)=O	dodecane	-5.89	-5.92		-10.82
2,4-octanedione	CCCCC(=O)CC(C)=O	dodecane	-6.47	-6.56		-11.90
2,4-nonanedione	CCCCCC(=O)CC(C)=O	dodecane	-7.22	-7.13		-12.64
3,5-octanedione	CCCC(=O)CC(=O)CC	dodecane	-6.51	-6.68		-12.11
4,6-nonanedione	CCCCC(=O)CC(=O)CCC	dodecane	-7.24	-7.19		-12.86
ethanol	CCO	dodecane	-2.06	-1.76		-4.61
1-propanol	CCCO	dodecane	-2.77	-2.57	-5.41	-5.95
1-butanol	CCCCO	dodecane	-3.53	-3.33		-7.21
1-pentanol	CCCCCO	dodecane	-4.24	-4.02		-8.31
1-hexanol	CCCCCCO	dodecane	-4.87	-4.92		-9.73
1-octanol	CCCCC(O)CCC	dodecane	-6.02	-6.01		-11.64
3-ethyl-3-hexanol	CCCC(O)(CC)CC	dodecane	-5.73	-5.56		-11.06
2-ethoxyethanol	CCOCCO	dodecane	-3.83	-4.26		-8.99
2-propoxyethanol	CCCOCCO	dodecane	-4.60	-4.99		-10.47
2-butoxyethanol	CCCCOCCO	dodecane	-5.27	-5.63		-11.18
2-pentoxyethanol	CCCCCOCCO	dodecane	-5.80	-6.27		-12.47
sulfur hexafluoride	F[S](F)(F)(F)(F)F	dodecane	0.07	-0.08		-1.65
trimethyl phosphate	CO[P](=O)(OC)OC	dodecane	-5.44	-5.49		-9.37
triethyl phosphate	CCO[P](=O)(OCC)OCC	dodecane	-6.21	-6.74		-11.07
tripropyl phosphate	CCCO[P](=O)(OCCC)OCCC	dodecane	-8.20	-8.12		-13.40
tributyl phosphate	O=P(OCCCC)(OCCCC)OCCCC	dodecane	-10.09	-9.55		-15.86
tetramethyl tin	C[Sn](C)(C)C	dodecane	-3.72	-3.61		-6.91
anisole	COc1ccccc1	dodecane	-5.27	-5.10		-9.49
acetophenone	CC(=O)c1ccccc1	dodecane	-6.11	-5.98		-10.81
nitrobenzene	[O-][N+](=O)c1ccccc1	dodecane	-6.07	-5.40		-10.06
benzyl alcohol	OCc1ccccc1	dodecane	-5.58	-5.80		-10.98
helium	[He]	hexadecane	2.38	1.64	1.97	1.48
neon	[Ne]	hexadecane	2.15	1.64	1.62	1.26
krypton	[Kr]	hexadecane	0.29	0.17	-1.20	-1.05
xenon	[Xe]	hexadecane	-0.52	-0.67	-2.41	-2.58
radon	[Rn]	hexadecane	-1.20	-0.72	-3.39	-2.57
methane	C	hexadecane	0.44	0.10	-0.95	-0.95
ethane	CC	hexadecane	-0.67	-0.67	-2.75	-2.43

propane	CCC	hexadecane	-1.43	-1.34	-3.81	-3.69
butane	CCCC	hexadecane	-2.20	-2.03	-4.97	-4.95
2-methylpropane	CC(C)C	hexadecane	-1.92	-1.93		-4.76
pentane	CCCCC	hexadecane	-2.95	-2.81	-6.20	-6.18
hexane	CCCCCC	hexadecane	-3.64	-3.56	-7.42	-7.37
heptane	CCCCCCC	hexadecane	-4.33	-4.29	-8.64	-8.48
nonane	CCCCCCCC	hexadecane	-5.70	-5.73		-10.73
decane	CCCCCCCCC	hexadecane	-6.39	-6.48		-11.92
undecane	CCCCCCCCC	hexadecane	-7.08	-7.13		-12.92
tridecane	CCCCCCCCCCC	hexadecane	-8.46	-8.54		-15.20
tetradecane	CCCCCCCCCCCC	hexadecane	-9.15	-9.20		-16.17
cyclopentane	C1CCCC1	hexadecane	-3.34	-3.38	-6.61	-7.09
cyclohexane	C1CCCCC1	hexadecane	-3.97	-4.10	-7.53	-8.20
2-methylpentane	CCCC(C)C	hexadecane	-3.42	-3.46		-7.18
2,2-dimethylpropane	CC(C)(C)C	hexadecane	-2.48	-2.25	-5.05	-5.28
2,4-dimethylpentane	CC(C)CC(C)C	hexadecane	-3.84	-4.06		-8.09
2,5-dimethylhexane	CC(C)CCC(C)C	hexadecane	-4.51	-4.81		-9.26
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	hexadecane	-4.64	-4.62		-8.98
propene	CC=C	hexadecane	-1.29	-1.23	-3.19	-3.54
pent-1-ene	CCCC=C	hexadecane	-2.75	-2.73		-5.96
hex-1-ene	CCCCC=C	hexadecane	-3.47	-3.51		-7.20
hept-1-ene	CCCCCC=C	hexadecane	-4.18	-4.23		-8.32
non-1-ene	CCCCCCC=C	hexadecane	-5.46	-5.72		-10.65
ethyne	C#C	hexadecane	-0.20	-0.68		-2.80
propyne	CC#C	hexadecane	-1.40	-1.30		-3.86
but-1-yne	C#CCC	hexadecane	-2.07	-2.01		-4.94
pent-1-yne	C#CCCC	hexadecane	-2.74	-2.75		-6.07
hex-1-yne	C#CCCCC	hexadecane	-3.42	-3.49		-7.18
hept-1-yne	C#CCCCC	hexadecane	-4.09	-4.18		-8.23
oct-1-yne	C#CCCCC	hexadecane	-4.75	-4.90		-9.33
non-1-yne	C#CCCCC	hexadecane	-5.40	-5.62		-10.42
benzene	c1ccccc1	hexadecane	-3.82	-3.62	-7.26	-7.26
ethylbenzene	CCc1ccccc1	hexadecane	-5.14	-5.08	-9.59	-9.55
propylbenzene	CCCc1ccccc1	hexadecane	-5.76	-5.83	-10.55	-10.71
butylbenzene	CCCCc1ccccc1	hexadecane	-6.39	-6.58		-11.88
pentylbenzene	CCCCC1ccccc1	hexadecane	-7.03	-7.32		-13.05
hexylbenzene	CCCCCc1ccccc1	hexadecane	-7.66	-8.00		-14.08
o-xylene	Cc1ccccc1C	hexadecane	-5.37	-4.97		-9.36
m-xylene	Cc1ccc(C)c1	hexadecane	-5.27	-5.01	-9.89	-9.44
p-xylene	Cc1cc(C)cc1	hexadecane	-5.26	-5.02	-9.92	-9.45
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	hexadecane	-6.00	-5.70	-11.13	-10.52
isopropylbenzene	CC(C)c1ccccc1	hexadecane	-5.60	-5.74		-10.55
naphthalene	c1ccc2ccccc2c1	hexadecane	-7.28	-6.65		-11.98
propanone	CC(C)=O	hexadecane	-2.40	-2.31		-5.33
butanone	CCC(C)=O	hexadecane	-3.92	-3.08		-6.52
pentan-2-one	CCCC(C)=O	hexadecane	-3.76	-3.78		-7.61
hexan-2-one	CCCCC(C)=O	hexadecane	-4.45	-4.53		-8.78
heptan-2-one	CCCCC(C)=O	hexadecane	-5.13	-5.18		-9.78
octan-2-one	CCCCC(C)=O	hexadecane	-5.81	-5.96		-10.99
nonan-2-one	CCCCC(C)=O	hexadecane	-6.49	-6.69		-12.14
pentan-3-one	CCC(=O)CC	hexadecane	-3.83	-3.82		-7.67
heptan-4-one	CCCC(=O)CCC	hexadecane	-5.21	-5.24		-9.90
4-methylpentan-2-one	CC(C)CC(C)=O	hexadecane	-4.16	-4.38		-8.53
cyclopentanone	O=C1CCCC1	hexadecane	-4.26	-4.41		-8.70
cyclohexanone	O=C1CCCCC1	hexadecane	-4.93	-5.10	-8.72	-9.76
acetophenone	CC(=O)c1ccccc1	hexadecane	-6.12	-5.95	-11.32	-10.86
formaldehyde	C=O	hexadecane	-1.00	-0.92		-3.03
acetaldehyde	CC=O	hexadecane	-1.68	-1.63		-4.31
propanal	CCC=O	hexadecane	-2.52	-2.47		-5.61
pentanal	CCCC=O	hexadecane	-3.78	-3.89		-7.76
hexanal	CCCCC=O	hexadecane	-4.60	-4.66		-8.97
heptanal	CCCCC=O	hexadecane	-5.27	-5.38		-10.10
octanal	CCCCC=O	hexadecane	-5.98	-5.95		-10.94
nonanal	CCCCC=O	hexadecane	-6.68	-6.81		-12.30
2-methylpropanal	CC(C)C=O	hexadecane	-2.81	-3.14		-6.64
benzaldehyde	O=Cc1ccccc1	hexadecane	-5.44	-5.28	-9.84	-9.85
(e)-but-2-enal	C/C=C/C=O	hexadecane	-3.51	-3.11		-6.63
diethyl ether	CCOCC	hexadecane	-2.81	-2.87	-6.02	-6.21
dipropyl ether	CCCOCC	hexadecane	-4.08	-4.33	-8.16	-8.50
di-isopropyl ether	CC(C)OC(C)C	hexadecane	-3.49	-3.96		-7.88
dibutyl ether	CCCCOCCCC	hexadecane	-5.46	-5.74	-10.38	-10.69
tetrahydropyran	C1CCOCC1	hexadecane	-4.08	-4.33		-8.64
methyl tert-butyl ether	COC(C)(C)C	hexadecane	-3.12	-3.05		-6.44
ethyl tert-butyl ether	CCOC(C)(C)C	hexadecane	-3.52	-3.70		-7.47
methyl tert-pentyl ether	CCC(C)(C)OC	hexadecane	-3.86	-3.72		-7.46
furan	c1ccccc1	hexadecane	-2.62	-3.11		-6.65
anisole	COc1ccccc1	hexadecane	-5.36	-5.06	-9.86	-9.51
phenetole	CCOc1ccccc1	hexadecane	-5.65	-5.77		-10.62
methyl formate	COC=O	hexadecane	-1.99	-1.98		-4.80
methyl acetate	COC(C)=O	hexadecane	-2.67	-2.52		-5.60
methyl propanoate	CCC(=O)OC	hexadecane	-3.35	-3.21		-6.68
methyl butanoate	CCCC(=O)OC	hexadecane	-4.01	-3.93		-7.81
methyl pentanoate	CCCCC(=O)OC	hexadecane	-4.70	-4.60		-8.84

methyl hexanoate	CCCCC(=O)OC	hexadecane	-5.43	-5.35		-10.01
ethyl formate	CCOC=O	hexadecane	-2.59	-2.51		-5.59
ethyl butanoate	CCCC(=O)OCC	hexadecane	-4.61	-4.55		-8.78
propyl formate	CCCOC=O	hexadecane	-3.29	-3.26		-6.78
propyl acetate	CCCOC(C)=O	hexadecane	-3.93	-3.83		-7.66
propyl butanoate	CCCCOC(=O)CCC	hexadecane	-5.20	-5.24		-9.87
butyl acetate	CCCCOC(C)=O	hexadecane	-4.61	-4.49	-9.20	-8.66
pentyl acetate	CCCCCOC(C)=O	hexadecane	-5.20	-5.19		-9.76
pentyl propanoate	CCCCCOC(=O)CC	hexadecane	-5.93	-5.90		-10.87
hexyl acetate	CCCCCOC(C)=O	hexadecane	-5.83	-5.88		-10.80
isopropyl formate	CC(C)OC=O	hexadecane	-3.04	-3.12		-6.54
isopropyl acetate	CC(C)OC(C)=O	hexadecane	-3.59	-3.66		-7.36
isopropyl propanoate	CCC(=O)OC(C)C	hexadecane	-4.13	-4.38		-8.50
isobutyl acetate	CC(C)COC(C)=O	hexadecane	-4.34	-4.41		-8.53
isoamyl formate	CC(C)CCOC=O	hexadecane	-4.57	-4.58		-8.79
isoamyl acetate	CC(C)CCOC(C)=O	hexadecane	-5.12	-5.13		-9.64
isobutyl isobutyrate	CC(C)COC(=O)C(C)C	hexadecane	-5.29	-5.66		-10.55
methyl benzoate	COC(=O)c1ccccc1	hexadecane	-6.32	-6.11	-11.56	-11.13
methanol	CO	hexadecane	-1.26	-1.15	-3.19	-3.53
ethanol	CCO	hexadecane	-2.03	-1.83	-3.90	-4.82
propan-1-ol	CCCO	hexadecane	-2.86	-2.57		-6.12
butan-1-ol	CCCCO	hexadecane	-3.55	-3.25		-7.17
pentan-1-ol	CCCCCO	hexadecane	-4.24	-4.06		-8.51
hexan-1-ol	CCCCCCO	hexadecane	-4.92	-4.73		-9.53
heptan-1-ol	CCCCCCCO	hexadecane	-5.61	-5.53	-10.62	-10.85
octan-1-ol	CCCCCCCCO	hexadecane	-6.30	-6.31		-12.05
decan-1-ol	CCCCCCCCCO	hexadecane	-7.68	-7.74		-14.32
butan-2-ol	CCC(C)O	hexadecane	-3.19	-3.15		-7.04
2-methylpropan-2-ol	CC(C)(C)O	hexadecane	-2.75	-2.99		-6.98
2-methylbutan-1-ol	CCC(C)CO	hexadecane	-4.11	-3.78		-8.00
3-methylbutan-1-ol	CC(C)CCO	hexadecane	-4.11	-3.90		-8.18
hexan-3-ol	CCCC(O)CC	hexadecane	-4.69	-4.55		-9.28
2-methylpentan-2-ol	CCCC(C)(C)O	hexadecane	-4.34	-4.28		-8.95
cyclohexanol	OC1CCCCC1	hexadecane	-5.01	-5.49	-11.36	-10.91
allyl alcohol	OCC=C	hexadecane	-2.72	-2.50		-5.95
benzyl alcohol	OCc1ccccc1	hexadecane	-6.06	-5.83	-10.13	-11.22
2-phenylethanol	OCCc1ccccc1	hexadecane	-6.21	-6.49		-12.21
3-phenylpropanol	OCCc1ccccc1	hexadecane	-6.55	-7.18		-13.33
4-phenylbutanol	OCCc1ccccc1	hexadecane	-6.85	-7.85		-14.37
phenol	Oc1ccccc1	hexadecane	-5.26	-5.01		-9.95
m-cresol	Cc1ccc(O)c1	hexadecane	-5.91	-5.77		-11.19
p-cresol	Cc1ccc(O)cc1	hexadecane	-5.88	-5.80		-11.25
2-nitrophenol	Oc1ccccc1[N+](=O)=O	hexadecane	-6.39	-5.71		-11.02
acetic acid	CC(O)=O	hexadecane	-2.39	-2.60		-6.25
propanoic acid	CCC(O)=O	hexadecane	-3.12	-3.39		-7.61
butanoic acid	CCCC(O)=O	hexadecane	-3.86	-4.04		-8.71
pentanoic acid	CCCCC(O)=O	hexadecane	-4.61	-4.73		-9.82
hexanoic acid	CCCCC(O)=O	hexadecane	-5.35	-5.36		-10.81
heptanoic acid	CCCCCCC(O)=O	hexadecane	-6.08	-6.12		-12.02
octanoic acid	CCCCCCCC(O)=O	hexadecane	-6.82	-6.83		-13.02
ammonia	N	hexadecane	-0.37	-0.13		-0.91
ethylamine	CCN	hexadecane	-2.29	-1.78		-4.40
propylamine	CCCN	hexadecane	-2.92	-2.44	-5.73	-5.65
pentylamine	CCCCCN	hexadecane	-4.21	-3.94	-8.32	-8.19
hexylamine	CCCCCN	hexadecane	-4.85	-4.61	-9.43	-9.44
heptylamine	CCCCCCN	hexadecane	-5.52	-5.37	-10.82	-10.72
tert-butylamine	CC(C)(C)N	hexadecane	-3.40	-2.82	-6.25	-6.92
dimethylamine	CNC	hexadecane	-2.18	-2.29		-5.67
diethylamine	CCNCC	hexadecane	-3.27	-3.50	-5.88	-7.87
dipropylamine	CCCNCCC	hexadecane	-4.60	-4.79		-10.06
di-isopropylamine	CC(C)NC(C)C	hexadecane	-3.95	-4.27		-9.32
trimethylamine	CN(C)C	hexadecane	-2.21	-2.43		-5.68
aniline	Nc1ccccc1	hexadecane	-5.45	-5.08	-9.99	-9.55
N,N-dimethylaniline	CN(C)c1ccccc1	hexadecane	-6.49	-5.91	-11.56	-10.90
pyridine	c1ccncc1	hexadecane	-4.10	-4.26	-7.80	-8.07
4-methylpyridine	Cc1ccncc1	hexadecane	-4.90	-5.00	-8.79	-9.25
2-ethylpyridine	CCc1cccn1	hexadecane	-5.32	-5.72		-10.46
3-ethylpyridine	CCc1cccn1	hexadecane	-5.63	-5.79		-10.55
4-ethylpyridine	CCc1ccncc1	hexadecane	-5.65	-5.77		-10.48
2,4-dimethylpyridine	Cc1ccncc(C)c1	hexadecane	-5.52	-5.64		-10.31
2,5-dimethylpyridine	Cc1ccc(C)nc1	hexadecane	-5.52	-5.68		-10.39
4-tert-butylpyridine	CC(C)(C)c1ccncc1	hexadecane	-6.48	-6.72		-12.01
nitromethane	C[N+](=O)=O	hexadecane	-2.58	-2.38	-6.06	-5.79
nitroethane	CC[N+](=O)=O	hexadecane	-3.23	-3.10		-6.95
1-nitropropane	CCC[N+](=O)=O	hexadecane	-3.89	-3.76		-7.95
1-nitrobutane	CCCC[N+](=O)=O	hexadecane	-4.54	-4.43		-8.97
1-nitropentane	CCCCC[N+](=O)=O	hexadecane	-5.21	-5.06		-9.89
2-nitropropane	CC(C)[N+](=O)=O	hexadecane	-3.48	-3.66	-7.21	-7.78
2-nitrotoluene	Cc1ccccc1[N+](=O)=O	hexadecane	-6.52	-6.29		-11.74
3-nitrotoluene	Cc1cccc(c1)[N+](=O)=O	hexadecane	-6.78	-6.23		-11.69
4-nitrotoluene	Cc1ccc(cc1)[N+](=O)=O	hexadecane	-6.85	-6.22		-11.66
acetoneitrile	CC#N	hexadecane	-2.13	-2.23	-4.56	-4.51
propanonitrile	CCC#N	hexadecane	-2.80	-2.94		-5.63

butanonitrile	CCCC#N	hexadecane	-3.46	-3.56		-6.58
pentanonitrile	CCCCC#N	hexadecane	-4.17	-4.11		-7.40
benzonitrile	N#Cc1ccccc1	hexadecane	-5.46	-5.45	-9.86	-9.40
chloromethane	CCl	hexadecane	-1.59	-1.60		-3.94
1-chloropropane	CCCCl	hexadecane	-3.00	-3.01		-6.52
1-chlorobutane	CCCCCl	hexadecane	-3.71	-3.69	-7.38	-7.57
1-chloropentane	CCCCCCL	hexadecane	-4.40	-4.41		-8.69
1-chlorohexane	CCCCCCCl	hexadecane	-5.06	-5.19		-9.93
2-chloropropane	CC(C)Cl	hexadecane	-2.69	-2.93		-6.39
2-chloro-2-methylpropane	CC(C)(C)Cl	hexadecane	-3.02	-3.39		-7.11
dichloromethane	ClCCl	hexadecane	-2.75	-2.77	-5.54	-5.83
trichloromethane	ClC(Cl)Cl	hexadecane	-3.38	-3.46		-6.76
1,2-dichloroethane	ClCCCl	hexadecane	-3.51	-3.81		-7.75
1,1-dichloroethane	CC(Cl)Cl	hexadecane	-3.21	-3.64		-7.46
1,1,2-trichloroethane	ClCC(Cl)Cl	hexadecane	-4.49	-4.76		-9.15
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	hexadecane	-5.22	-5.38		-9.89
1,3-dichloropropane	ClCCCCl	hexadecane	-4.36	-4.52		-8.86
1,4-dichlorobutane	ClCCCCCl	hexadecane	-5.15	-5.41		-10.23
bromoethane	CCBr	hexadecane	-2.76	-2.91		-6.48
1-bromopropane	CCCBBr	hexadecane	-3.57	-3.60		-7.54
1-bromobutane	CCCCBr	hexadecane	-4.24	-4.25		-8.53
1-bromopentane	CCCCCBr	hexadecane	-4.93	-4.89		-9.52
1-bromoheptane	CCCCCCBr	hexadecane	-6.28	-6.12		-11.37
2-bromopropane	CC(C)Br	hexadecane	-3.26	-3.52		-7.41
1-bromo-2-methylpropane	CC(C)CBr	hexadecane	-4.04	-4.14		-8.35
tribromomethane	BrC(Br)Br	hexadecane	-5.11	-5.12		-9.84
1,2-dibromoethane	BrCCBr	hexadecane	-5.46	-5.13		-10.02
iodoethane	CCl	hexadecane	-3.51	-3.50		-6.77
1-iodopropane	CCCI	hexadecane	-4.27	-4.17		-7.81
1-iodobutane	CCCCI	hexadecane	-4.95	-4.89		-8.92
1-iodopentane	CCCCCI	hexadecane	-5.63	-5.66		-10.12
1-iodoheptane	CCCCCCI	hexadecane	-6.94	-6.82		-11.81
diiodomethane	ICI	hexadecane	-5.26	-5.45	-9.31	-9.24
2-bromo-2-chloro-1,1,1-trifluoroethane	FC(F)(F)C(Cl)Br	hexadecane	-2.97	-3.09		-6.75
2-chloro-2-(difluoromethoxy)-1,1,1-trifluoro-ethane	FC(F)OC(Cl)C(F)(F)F	hexadecane	-2.15	-2.67		-6.78
2,2,2-trifluoroethyl vinyl ether	FC(F)(F)COC=C	hexadecane	-1.91	-2.20		-5.82
1,1-dichloroethene	ClC(Cl)=C	hexadecane	-2.88	-2.83		-6.03
cis-1,2-dichloroethene	ClC=C(Cl)	hexadecane	-3.34	-2.95		-6.24
trans-1,2-dichloroethene	ClC=C(Cl)	hexadecane	-3.21	-3.27		-6.84
trichloroethene	ClC=C(Cl)Cl	hexadecane	-4.09	-3.76		-7.48
allyl chloride	CICC=C	hexadecane	-2.88	-2.94		-6.39
allyl bromide	BrCC=C	hexadecane	-3.42	-3.56		-7.43
allyl iodide	ICC=C	hexadecane	-4.11	-4.00		-7.44
fluorobenzene	Fc1ccccc1	hexadecane	-3.87	-3.58	-7.42	-7.26
chlorobenzene	Clc1ccccc1	hexadecane	-4.97	-4.98	-9.14	-9.47
2-chlorotoluene	Cc1ccccc1Cl	hexadecane	-5.67	-5.73		-10.62
1,2-dichlorobenzene	Clc1ccccc1Cl	hexadecane	-6.01	-5.99		-10.99
1,3-dichlorobenzene	Clc1cccc(Cl)c1	hexadecane	-5.99	-6.31		-11.60
bromobenzene	Brc1ccccc1	hexadecane	-5.50	-5.50		-10.35
2-bromotoluene	Cc1ccccc1Br	hexadecane	-6.17	-6.21		-11.44
4-bromotoluene	Cc1ccc(Br)cc1	hexadecane	-6.19	-6.22		-11.47
1-propanethiol	CCCS	hexadecane	-3.66	-3.52		-6.65
1-butanethiol	CCCCS	hexadecane	-3.93	-4.27		-8.08
dimethyl sulfide	CSC	hexadecane	-3.05	-2.29		-4.51
diethyl sulfide	CCSCC	hexadecane	-4.23	-3.96		-7.64
dipropyl sulfide	CCSCCC	hexadecane	-5.62	-5.31		-9.65
di-isopropyl sulfide	CC(C)SC(C)C	hexadecane	-4.91	-5.20		-9.46
dimethyl disulfide	CSSC	hexadecane	-4.84	-4.57		-7.72
dimethyl sulfoxide	C[S](C)=O	hexadecane	-4.24	-5.36		-10.68
thiophene	s1ccccc1	hexadecane	-4.01	-3.91	-7.15	-7.35
2-methylthiophene	Cc1sccc1	hexadecane	-4.50	-4.64		-8.61
thiophenol	Sc1ccccc1	hexadecane	-5.62	-5.87		-10.64
dimethylformamide	CN(C)C=O	hexadecane	-3.99	-4.09		-8.61
dimethylacetamide	CN(C)C(C)=O	hexadecane	-4.58	-4.63		-9.47
helium	[He]	methylcyclohexane	2.06	1.92		1.87
neon	[Ne]	methylcyclohexane	1.86	1.78		1.54
argon	[Ar]	methylcyclohexane	0.61	0.54		-0.21
krypton	[Kr]	methylcyclohexane	-0.05	-0.06		-1.01
xenon	[Xe]	methylcyclohexane	-0.87	-0.95		-2.40
oxygen	O=O	methylcyclohexane	0.70	0.87		0.28
nitrogen	N#N	methylcyclohexane	1.01	0.95		0.85
carbon monoxide	[C-]#[O+]	methylcyclohexane	0.86	0.74		0.10
carbon dioxide	O=C=O	methylcyclohexane	-0.34	0.08		-0.89
methane	C	methylcyclohexane	0.16	0.12		-0.81
cyclohexane	C1CCCCC1	methylcyclohexane	-4.32	-4.14		-7.31
methylcyclohexane	CC1CCCCC1	methylcyclohexane	-4.77	-4.71		-8.18
ethylcyclohexane	CCC1CCCCC1	methylcyclohexane	-5.52	-5.44		-9.32
carbon tetrafluoride	FC(F)(F)F	methylcyclohexane	0.79	0.77		-0.14
methyl tert-pentyl ether	CCC(C)(C)OC	methylcyclohexane	-4.41	-4.22		-7.64
1,4-dioxane	C1COCCO1	methylcyclohexane	-4.01	-4.43		-8.00
acetone	CC(C)=O	methylcyclohexane	-2.58	-2.86		-5.47



methoxyacetone	COCC(C)=O	methylcyclohexane	-3.55	-3.87		-7.02
dimethyl carbonate	COC(=O)OC	methylcyclohexane	-3.62	-3.78		-7.11
propionitrile	CCC#N	methylcyclohexane	-3.56	-3.53		-5.89
butyronitrile	CCCC#N	methylcyclohexane	-4.26	-4.19		-6.94
ethanol	CCO	methylcyclohexane	-2.58	-2.32		-4.86
1-propanol	CCCO	methylcyclohexane	-3.42	-3.10		-6.13
1-butanol	CCCCO	methylcyclohexane	-4.17	-3.81		-7.31
isobutanol	CC(C)CO	methylcyclohexane	-3.94	-3.79		-7.27
2-butanol	CCC(C)O	methylcyclohexane	-3.86	-3.72		-7.19
2-methyl-isopropanol	CC(C)(C)O	methylcyclohexane	-3.49	-3.53		-7.04
sulfur hexafluoride	F[S](F)(F)(F)(F)F	methylcyclohexane	-0.18	0.01		-1.29
toluene	Cc1ccccc1	methylcyclohexane	-4.84	-4.82		-8.59
ethylbenzene	CCc1ccccc1	methylcyclohexane	-5.48	-5.55		-9.70
helium	[He]	tetradecane	2.18	1.74	1.41	1.60
neon	[Ne]	tetradecane	2.02	1.66	1.41	1.30
argon	[Ar]	tetradecane	0.80	0.68	-0.35	-0.19
krypton	[Kr]	tetradecane	0.17	0.21	-1.27	-1.10
nitrogen	N#N	tetradecane	1.24	1.11		0.56
oxygen	O=O	tetradecane	0.89	0.71		-0.08
sulfur hexafluoride	F[S](F)(F)(F)(F)F	tetradecane	0.16	-0.09		-1.57
methane	C	tetradecane	0.36	0.18		-0.94
methanol	CO	tetradecane	-1.20	-1.01		-3.22
1-propanol	CCCO	tetradecane	-2.65	-2.53		-5.91
1-butanol	CCCCO	tetradecane	-3.36	-3.29		-7.17
benzene	c1ccccc1	tetradecane	-3.81	-3.69	-7.31	-7.45
helium	[He]	pentadecane	2.19	1.71		1.58
neon	[Ne]	pentadecane	2.01	1.65		1.28
argon	[Ar]	pentadecane	0.82	0.66		-0.21
krypton	[Kr]	pentadecane	0.18	0.19		-1.08
nitrogen	N#N	pentadecane	1.27	1.11		0.58
oxygen	O=O	pentadecane	0.92	0.71		-0.03
tetrafluoromethane	FC(F)(F)F	pentadecane	1.11	0.67		-0.33
methane	C	pentadecane	0.38	0.15		-0.96
helium	[He]	cyclooctane	2.49	1.95		1.89
neon	[Ne]	cyclooctane	2.19	1.78		1.54
argon	[Ar]	cyclooctane	0.86	0.75		-0.03
nitrogen	N#N	cyclooctane	1.32	0.98		0.53
oxygen	O=O	cyclooctane	0.97	0.86		-0.11
carbon monoxide	[C-]#[O+]	cyclooctane	1.11	1.07		0.32
carbon dioxide	O=C=O	cyclooctane	-0.13	0.01		-1.52
methane	C	cyclooctane	0.41	0.38		-0.64
tetrafluoromethane	FC(F)(F)F	cyclooctane	1.25	1.11		0.21
helium	[He]	cyclohexane	2.13	1.95	2.42	1.91
neon	[Ne]	cyclohexane	1.88	1.80	1.46	1.57
argon	[Ar]	cyclohexane	0.65	0.50	-0.22	-0.22
krypton	[Kr]	cyclohexane	-0.04	-0.10	-0.85	-0.99
xenon	[Xe]	cyclohexane	-1.00	-1.05	-2.39	-2.49
hydrogen	[H][H]	cyclohexane	1.41	1.45	1.24	1.08
carbon dioxide	O=C=O	cyclohexane	-0.32	-0.10	-1.59	-1.17
sulfur hexafluoride	F[S](F)(F)(F)(F)F	cyclohexane	-0.12	-0.02	-1.38	-1.35
methane	C	cyclohexane	0.18	0.07	-0.72	-0.79
ethane	CC	cyclohexane	-0.98	-0.82	-2.66	-2.21
n-butane	CCCC	cyclohexane	-2.86	-2.43		-4.76
n-pentane	CCCCC	cyclohexane	-3.32	-3.19		-5.95
2-methylpentane	CCCC(C)C	cyclohexane	-3.86	-3.74	-6.91	-6.78
n-octane	CCCCCCCC	cyclohexane	-5.51	-5.32		-9.31
2,5-dimethylhexane	CC(C)CCC(C)C	cyclohexane	-5.01	-5.04		-8.81
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	cyclohexane	-5.10	-4.90		-8.61
n-nonane	CCCCCCCCC	cyclohexane	-6.27	-5.99		-10.31
cyclohexane	C1CCCCC1	cyclohexane	-4.43	-4.18	-7.90	-7.28
ethylcyclohexane	CCC1CCCCC1	cyclohexane	-5.60	-5.50		-9.35
ethyne	C#C	cyclohexane	-0.45	-0.83		-2.21
trichloromethane	ClC(Cl)Cl	cyclohexane	-3.45	-3.73	-6.75	-6.59
1,2-dichloroethane	ClCCCl	cyclohexane	-3.83	-3.92		-6.91
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	cyclohexane	-5.57	-5.82		-9.70
1,3-dichloropropane	ClCCCCl	cyclohexane	-4.47	-4.65		-8.07
1-chlorobutane	CCCCCl	cyclohexane	-4.28	-3.96	-7.32	-7.11
2-chloro-2-methylpropane	CC(C)(C)Cl	cyclohexane	-3.65	-3.73	-6.39	-6.77
trichloroethene	C1C=C(Cl)Cl	cyclohexane	-4.34	-4.24	-7.70	-7.50
tetrachloroethene	ClC(Cl)=C(Cl)Cl	cyclohexane	-5.18	-4.87		-8.54
chlorotrifluoromethane	FC(F)(F)Cl	cyclohexane	-0.49	-0.45	-2.22	-2.18
diethylether	CCOCC	cyclohexane	-2.66	-3.38		-6.27
dipropyl ether	CCCOCCC	cyclohexane	-4.57	-4.72	-8.15	-8.33
di-n-butylether	CCCCOCCCC	cyclohexane	-6.04	-6.05		-10.39
methyl butyl ether	CCCCOC	cyclohexane	-3.93	-4.14		-7.46
methyl t-butyl ether	COC(C)(C)C	cyclohexane	-3.64	-3.61		-6.59
ethyl t-butyl ether	CCOC(C)(C)C	cyclohexane	-4.12	-4.18		-7.46
dimethoxymethane	COCOC	cyclohexane	-2.95	-3.37	-5.67	-6.26
diethoxymethane	CCOCCOC	cyclohexane	-4.37	-4.42		-7.78
1,2-diethoxyethane	CCOCCOCC	cyclohexane	-4.64	-5.21		-9.00
diglyme	COCOCOCOC	cyclohexane	-5.63	-6.04		-10.44
tetrahydrofuran	C1CCOC1	cyclohexane	-4.48	-4.16	-6.86	-7.63
furan	o1ccccc1	cyclohexane	-2.93	-3.65		-6.73

butanal	CCCC=O	cyclohexane	-3.48	-3.75		-6.79
butanone	CCC(C)=O	cyclohexane	-3.36	-3.77		-6.86
hexan-2-one	CCCCC(C)=O	cyclohexane	-4.82	-5.20		-9.13
hexan-3-one	CCCC(=O)CC	cyclohexane	-4.83	-5.21		-9.18
heptan-2-one	CCCCCC(C)=O	cyclohexane	-5.50	-5.88		-10.24
cyclopentanone	O=C1CCCC1	cyclohexane	-4.63	-4.87	-8.04	-8.55
cyclohexanone	O=C1CCCCC1	cyclohexane	-5.36	-5.53	-9.00	-9.53
methyl acetate	COC(C)=O	cyclohexane	-2.81	-3.51	-5.72	-6.61
ethyl acetate	CCOC(C)=O	cyclohexane	-3.41	-4.05	-6.66	-7.43
butyl acetate	CCCCOC(C)=O	cyclohexane	-5.03	-5.32	-8.94	-9.42
pentyl acetate	CCCCCOC(C)=O	cyclohexane	-5.77	-5.96		-10.40
methyl propanoate	CCC(=O)OC	cyclohexane	-3.71	-4.11	-6.60	-7.52
methyl pentanoate	CCCCC(=O)OC	cyclohexane	-5.03	-5.38		-9.49
acetonitrile	CC#N	cyclohexane	-1.90	-2.99	-4.29	-5.04
n-propylamine	CCCN	cyclohexane	-3.06	-2.90		-5.72
n-butylamine	CCCCN	cyclohexane	-3.85	-3.73	-7.05	-7.04
trimethylamine	CN(C)C	cyclohexane	-2.61	-3.03		-5.99
triethylamine	CCN(CC)CC	cyclohexane	-4.72	-4.72	-8.08	-8.77
nitromethane	C[N+](=O)=O	cyclohexane	-2.76	-3.06	-6.12	-6.13
nitropropane	CCC[N+](=O)=O	cyclohexane	-4.07	-4.44		-8.30
ethanol	CCO	cyclohexane	-2.25	-2.43	-4.18	-4.97
propan-1-ol	CCCO	cyclohexane	-2.82	-3.16		-6.13
butan-1-ol	CCCCO	cyclohexane	-3.53	-3.84		-7.25
2-methylpropan-1-ol	CC(C)CO	cyclohexane	-3.34	-3.71		-7.04
butan-2-ol	CCC(C)O	cyclohexane	-3.31	-3.75		-7.13
2-methylpropan-2-ol	CC(C)(C)O	cyclohexane	-2.91	-3.58		-7.03
pentan-1-ol	CCCCCO	cyclohexane	-4.22	-4.59		-8.47
hexan-1-ol	CCCCCCO	cyclohexane	-5.02	-5.29		-9.61
heptan-1-ol	CCCCCCCO	cyclohexane	-5.74	-6.06		-10.87
2-methoxyethanol	COCCO	cyclohexane	-4.90	-4.07	-7.78	-8.11
methanethiol	CS	cyclohexane	-2.63	-2.21		-3.59
methyl ethyl sulfide	CCSC	cyclohexane	-3.86	-3.85		-6.52
benzene	c1ccccc1	cyclohexane	-4.07	-4.24	-7.33	-7.64
toluene	Cc1ccccc1	cyclohexane	-4.89	-4.89	-8.38	-8.64
chlorobenzene	Clc1ccccc1	cyclohexane	-5.39	-5.29	-8.89	-9.16
anisole	COc1ccccc1	cyclohexane	-5.44	-5.61	-9.47	-9.66
phenetole	CCOc1ccccc1	cyclohexane	-6.00	-6.22		-10.57
benzaldehyde	O=Cc1ccccc1	cyclohexane	-5.57	-5.83	-9.54	-9.95
methyl benzoate	COC(=O)c1ccccc1	cyclohexane	-6.77	-6.99	-11.19	-11.94
benzonitrile	N#Cc1ccccc1	cyclohexane	-5.73	-6.36	-9.74	-10.23
o-toluidine	Cc1ccccc1N	cyclohexane	-6.37	-6.40		-11.05
p-toluidine	Cc1ccc(N)cc1	cyclohexane	-6.34	-6.57		-11.16
2-chloroaniline	Nc1ccccc1Cl	cyclohexane	-6.51	-7.31		-12.33
3-chloroaniline	Nc1cccc(Cl)c1	cyclohexane	-7.04	-7.29		-12.38
4-chloroaniline	Nc1ccc(Cl)cc1	cyclohexane	-6.85	-7.27		-12.34
2-methoxyaniline	COc1ccccc1N	cyclohexane	-6.83	-8.18		-14.50
3-methoxyaniline	COc1cccc(N)c1	cyclohexane	-7.12	-8.35		-14.78
2-nitroaniline	Nc1ccccc1[N+](=O)=O	cyclohexane	-7.87	-8.34		-14.87
3-nitroaniline	Nc1cccc(c1)[N+](=O)=O	cyclohexane	-8.28	-8.77		-15.87
n-methylaniline	CNc1ccccc1	cyclohexane	-6.30	-6.33	-10.42	-11.04
N,N-dimethylaniline	CN(C)c1ccccc1	cyclohexane	-6.82	-6.76	-11.09	-11.76
nitrobenzene	[O-][N+](=O)c1ccccc1	cyclohexane	-6.43	-6.17	-10.30	-10.86
phenol	Oc1ccccc1	cyclohexane	-5.52	-5.30		-9.28
o-cresol	Cc1ccccc1O	cyclohexane	-5.83	-5.89		-10.23
m-cresol	Cc1cccc(O)c1	cyclohexane	-5.81	-5.96		-10.30
p-cresol	Cc1ccc(O)cc1	cyclohexane	-5.66	-5.98		-10.34
2,3-dimethylphenol	Cc1ccc(O)c(C)c1	cyclohexane	-6.86	-6.58		-11.33
2,4-dimethylphenol	Cc1ccc(O)c(C)c1	cyclohexane	-6.82	-6.54		-11.24
2,6-dimethylphenol	Cc1ccc(C)c(C)c1O	cyclohexane	-6.63	-6.53		-11.30
3,4-dimethylphenol	Cc1ccc(O)cc(C)c1	cyclohexane	-6.85	-6.59		-11.28
benzyl alcohol	OCc1ccccc1	cyclohexane	-5.78	-6.09		-10.56
pyridine	c1ccncc1	cyclohexane	-4.27	-4.75	-7.65	-8.03
2-methylpyridine	Cc1cccn1	cyclohexane	-4.95	-5.49	-8.59	-9.25
3-methylpyridine	Cc1ccnc1	cyclohexane	-5.14	-5.49	-8.63	-9.22
4-methylpyridine	Cc1ccncc1	cyclohexane	-5.22	-5.49	-8.87	-9.21
2,4-dimethylpyridine	Cc1ccnc(C)c1	cyclohexane	-5.78	-6.21	-9.53	-10.42
2,6-dimethylpyridine	Cc1cccc(C)n1	cyclohexane	-5.47	-6.19	-9.53	-10.45
3,5-dimethylpyridine	Cc1cnc(C)cc1	cyclohexane	-5.88	-6.22		-10.40
water	O	cyclohexane	-0.51	-1.35		-3.55
helium	[He]	acetone	1.98	2.09	2.75	2.16
neon	[Ne]	acetone	1.75	1.92	2.41	1.83
argon	[Ar]	acetone	0.71	0.70	0.46	0.01
krypton	[Kr]	acetone	0.10	0.13		-0.59
xenon	[Xe]	acetone	-0.68	-0.90		-2.26
radon	[Rn]	acetone	-1.02	-1.07	-2.51	-2.47
hydrogen	[H][H]	acetone	1.36	1.44	1.08	0.98
oxygen	O=O	acetone	0.76	1.09	0.03	0.55
nitrogen	N#N	acetone	1.02	0.95	0.42	0.79
nitrous oxide	[O-][N+]=N	acetone	-1.05	-0.98		-2.23
carbon monoxide	[C-]#[O+]	acetone	0.80	0.45	0.06	-0.29
carbon dioxide	O=C=O	acetone	-1.08	-0.91		-2.62
sulfur dioxide	O=[S]=O	acetone	-3.52	-2.93		-6.52
hydrogen sulfide	S	acetone	-1.90	-1.89		-3.29

methane	C	acetone	0.30	0.10	-0.67	-0.85
ethane	CC	acetone	-0.68	-0.77	-2.06	-2.27
pentane	CCCCC	acetone	-2.70	-2.60	-4.68	-5.08
2,2-dimethylpropane	CC(C)(C)C	acetone	-2.22	-2.01		-4.13
hexane	CCCCCC	acetone	-3.23	-3.22	-5.77	-6.01
octane	CCCCCCCC	acetone	-4.41	-4.58	-7.59	-8.23
2-methylpentane	CCCC(C)C	acetone	-3.06	-3.03		-5.70
2,4-dimethylpentane	CC(C)CC(C)C	acetone	-3.44	-3.50		-6.45
2,5-dimethylhexane	CC(C)CCC(C)C	acetone	-4.02	-4.16		-7.48
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	acetone	-4.13	-3.94		-7.24
cyclohexane	C1CCCCC1	acetone	-3.55	-3.50	-6.25	-5.98
methylcyclohexane	CC1CCCCC1	acetone	-3.93	-3.89		-6.51
ethylcyclohexane	CCC1CCCCC1	acetone	-4.53	-4.54		-7.49
ethene	C=C	acetone	-0.76	-1.24		-3.02
isobutene	CC(C)=C	acetone	-2.37	-2.29		-4.57
1,3-butadiene	C=CC=C	acetone	-2.74	-2.84		-5.45
ethyne	C#C	acetone	-1.83	-1.64		-3.53
propyne	CC#C	acetone	-2.48	-2.18		-4.27
1-butyne	CCC#C	acetone	-2.99	-2.80		-5.23
trichloromethane	ClC(Cl)Cl	acetone	-4.65	-4.44		-7.98
tetrachloromethane	ClC(Cl)(Cl)Cl	acetone	-4.15	-4.49	-7.64	-8.04
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	acetone	-6.28	-6.91	-12.73	-11.75
1,3-dichloropropane	ClCCCCl	acetone	-5.63	-5.08		-8.77
1-chlorobutane	CCCCCl	acetone	-4.26	-4.10	-7.55	-7.45
1,4-dichlorobutane	ClCCCCCl	acetone	-6.56	-6.04		-10.24
1-chloropentane	CCCCC1	acetone	-4.86	-4.71		-8.37
2-bromo-2-methylpropane	CC(C)(C)Br	acetone	-3.86	-3.79	-7.07	-6.96
iodomethane	CI	acetone	-3.55	-3.16	-6.37	-5.45
iodoethane	CCI	acetone	-3.98	-3.80		-6.46
1,2-difluorotetrachloroethane	FC(Cl)(Cl)C(F)(Cl)Cl	acetone	-4.45	-5.06		-9.45
halothane	FC(F)(F)C(Cl)Br	acetone	-4.77	-3.90		-7.27
diethylether	CCOCC	acetone	-3.25	-3.39		-6.01
1,4-dioxane	C1COCCO1	acetone	-5.07	-4.81	-9.13	-8.02
propanone	CC(C)=O	acetone	-4.15	-3.83		-6.93
butanone	CCC(C)=O	acetone	-4.67	-4.37		-7.67
methyl acetate	COC(C)=O	acetone	-4.12	-4.38		-7.59
ammonia	N	acetone	-2.02	-2.87		-6.13
diethylamine	CCNCC	acetone	-3.75	-4.48		-9.27
trimethylamine	CN(C)C	acetone	-2.56	-3.01		-5.92
triethylamine	CCN(CC)CC	acetone	-4.05	-4.28	-7.24	-8.33
nitromethane	C[N+](=O)[O-]	acetone	-5.29	-4.77	-9.33	-8.94
dimethylformamide	CN(C)C=O	acetone	-6.43	-5.90	-11.40	-10.78
methanol	CO	acetone	-4.13	-4.04	-8.10	-8.79
ethanol	CCO	acetone	-4.42	-4.52	-9.00	-9.57
cyclopentanol	OC1CCCC1	acetone	-6.28	-6.76		-12.74
cyclohexanol	OC1CCCCC1	acetone	-6.94	-7.16		-13.27
tetraethylsilicon	CC[Si](CC)(CC)CC	acetone	-5.24	-5.35		-9.05
tetramethylstannane	C[Sn](C)(C)C	acetone	-3.48	-3.67	-6.05	-5.90
tetraethyltin	CC[Sn](CC)(CC)CC	acetone	-6.17	-5.74	-9.68	-9.19
benzene	c1ccccc1	acetone	-4.38	-4.29	-7.49	-7.52
isopropylbenzene	CC(C)c1ccccc1	acetone	-5.89	-6.10		-10.33
isopropenylbenzene	CC(=C)c1ccccc1	acetone	-6.37	-6.28		-10.58
aniline	Nc1ccccc1	acetone	-7.84	-7.81	-13.92	-13.73
pyridine	c1ccncc1	acetone	-5.42	-5.95		-9.63
water	O	acetone	-4.39	-4.22	-9.48	-9.87
hydrogen	[H][H]	methyl ethyl ketone	1.45	1.48		0.98
oxygen	O=O	methyl ethyl ketone	0.76	1.12		0.53
ammonia	N	methyl ethyl ketone	-1.94	-2.88		-6.23
butane	CCCC	methyl ethyl ketone	-2.31	-2.09		-4.43
hexane	CCCCCC	methyl ethyl ketone	-3.44	-3.36	-6.35	-6.37
2-methylpentane	CCCC(C)C	methyl ethyl ketone	-3.26	-3.18		-6.11
2,4-dimethylpentane	CC(C)CC(C)C	methyl ethyl ketone	-3.66	-3.66		-6.89
octane	CCCCCCCC	methyl ethyl ketone	-4.71	-4.77	-8.43	-8.74
2,5-dimethylhexane	CC(C)CCC(C)C	methyl ethyl ketone	-4.28	-4.34		-7.97
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	methyl ethyl ketone	-4.05	-3.87		-7.30
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	methyl ethyl ketone	-4.39	-4.11		-7.69
nonane	CCCCCCCCC	methyl ethyl ketone	-5.32	-5.35		-9.55
decane	CCCCCCCCCC	methyl ethyl ketone	-6.03	-6.00	-10.50	-10.55
cyclohexane	C1CCCCC1	methyl ethyl ketone	-3.75	-3.62	-6.74	-6.30
methylcyclohexane	CC1CCCCC1	methyl ethyl ketone	-4.12	-4.01	-7.31	-6.84
ethylcyclohexane	CCC1CCCCC1	methyl ethyl ketone	-4.82	-4.66		-7.82
propylene	CC=C	methyl ethyl ketone	-1.54	-1.82		-3.93
2-methylbuta-1,3-diene	CC(=C)C=C	methyl ethyl ketone	-3.27	-3.16		-5.91
pent-1-ene	CCCC=C	methyl ethyl ketone	-2.88	-3.09		-5.92
isopentene	CC(C)C=C	methyl ethyl ketone	-2.71	-2.88		-5.53
cyclohexene	C1CCC=CC1	methyl ethyl ketone	-4.00	-4.08	-7.28	-7.21
1,4-cyclohexadiene	C1C=CCC=C1	methyl ethyl ketone	-4.41	-4.27		-7.54
dichloromethane	ClCCl	methyl ethyl ketone	-4.05	-3.52		-6.54
trichloromethane	ClC(Cl)Cl	methyl ethyl ketone	-4.72	-4.36		-7.89
tetrachloromethane	ClC(Cl)(Cl)Cl	methyl ethyl ketone	-4.15	-4.39	-7.99	-7.99
2-chloro-2-methylpropane	CC(C)(C)Cl	methyl ethyl ketone	-3.66	-3.47		-6.44
1,2-dichloroethane	ClCCCl	methyl ethyl ketone	-4.79	-4.45	-7.75	-7.90
bromoethane	CCBr	methyl ethyl ketone	-3.53	-3.10		-5.99

iodomethane	CI	methyl ethyl ketone	-3.48	-3.11		-5.45
iodoethane	CCI	methyl ethyl ketone	-4.07	-3.75		-6.45
1,1,2-trichlorotrifluoroethane	FC(F)(Cl)C(F)(Cl)Cl	methyl ethyl ketone	-3.36	-3.64		-7.50
tetrachloroethene	ClC(Cl)=C(Cl)Cl	methyl ethyl ketone	-4.98	-4.62		-8.41
dipropyl ether	CCCOC	methyl ethyl ketone	-4.37	-4.51		-7.82
diisopropyl ether	CC(C)OC(C)C	methyl ethyl ketone	-3.90	-3.93		-6.93
1,4-dioxane	C1COCCO1	methyl ethyl ketone	-5.02	-4.68	-6.74	-7.86
ethyl formate	CCOC=O	methyl ethyl ketone	-3.71	-3.83		-6.68
ethyl acetate	CCOC(C)=O	methyl ethyl ketone	-4.49	-4.39		-7.60
propionaldehyde	CCC=O	methyl ethyl ketone	-3.85	-3.81		-6.81
propanone	CC(C)=O	methyl ethyl ketone	-3.98	-3.68		-6.68
butanone	CCC(C)=O	methyl ethyl ketone	-4.58	-4.29	-8.32	-7.58
nitromethane	C[N+](=O)=O	methyl ethyl ketone	-4.98	-4.58		-8.62
nitroethane	CC[N+](=O)=O	methyl ethyl ketone	-5.25	-5.25		-9.61
acetonitrile	CC#N	methyl ethyl ketone	-4.46	-4.77	-7.99	-7.77
triethylamine	CCN(CC)CC	methyl ethyl ketone	-4.16	-4.34		-8.57
methanol	CO	methyl ethyl ketone	-3.83	-3.95	-8.13	-8.72
ethanol	CCO	methyl ethyl ketone	-4.32	-4.43	-8.68	-9.51
propan-1-ol	CCCO	methyl ethyl ketone	-4.97	-5.09		-10.53
propan-2-ol	CC(C)O	methyl ethyl ketone	-4.54	-4.84		-10.11
butan-1-ol	CCCCO	methyl ethyl ketone	-5.66	-5.56		-11.17
2-butanol	CCC(C)O	methyl ethyl ketone	-5.18	-5.26	-10.22	-10.63
isobutanol	CC(C)CO	methyl ethyl ketone	-5.43	-5.64	-10.85	-11.40
2-methyl-isopropanol	CC(C)(C)O	methyl ethyl ketone	-4.71	-4.51	-9.62	-9.37
1-octanol	CCCCCCCCO	methyl ethyl ketone	-8.20	-8.14	-15.11	-15.19
acetic acid	CC(=O)O	methyl ethyl ketone	-5.42	-6.40		-12.94
benzene	c1ccccc1	methyl ethyl ketone	-4.49	-4.21	-8.14	-7.40
toluene	Cc1ccccc1	methyl ethyl ketone	-5.10	-4.84	-9.13	-8.42
ethylbenzene	CCc1ccccc1	methyl ethyl ketone	-5.65	-5.49	-10.02	-9.40
carbon disulfide	S=C=S	methyl ethyl ketone	-3.10	-3.02		-3.75
pyridine	c1ccncc1	methyl ethyl ketone	-5.37	-5.86		-9.56
oxygen	O=O	2-pentanone	0.81	1.09		0.47
2-pentanone	CCCC(C)=O	2-pentanone	-5.03	-4.82		-8.49
2-heptanone	CCCCC(C)=O	2-heptanone	-6.17	-5.83		-10.07
pentane	CCCCC	methyl isobutyl ketone	-2.86	-2.86		-5.81
hexane	CCCCCC	methyl isobutyl ketone	-3.59	-3.60		-7.00
heptane	CCCCCCC	methyl isobutyl ketone	-4.36	-4.28		-8.05
cyclohexane	C1CCCCC1	methyl isobutyl ketone	-3.92	-3.84		-6.90
benzene	c1ccccc1	methyl isobutyl ketone	-4.44	-4.32		-7.80
tetrachloromethane	ClC(Cl)(Cl)Cl	methyl isobutyl ketone	-4.22	-4.19		-7.69
1,2-dichloroethane	ClCCCl	methyl isobutyl ketone	-4.68	-4.53		-8.25
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	methyl isobutyl ketone	-4.28	-5.32		-9.46
helium	[He]	cyclohexanone	2.46	2.10	2.58	2.18
argon	[Ar]	cyclohexanone	1.05	1.06	0.16	0.32
krypton	[Kr]	cyclohexanone	0.37	0.47	-0.81	-0.44
hydrogen	[H][H]	cyclohexanone	1.75	1.59	1.38	1.13
deuterium	[H][H]	cyclohexanone	1.73	1.59	1.30	1.13
oxygen	O=O	cyclohexanone	1.13	0.99	0.26	-0.10
sulfur hexafluoride	F[S](F)(F)(F)(F)F	cyclohexanone	0.52	0.56	-0.98	-0.85
carbon dioxide	O=C=O	cyclohexanone	-0.79	-0.55	-3.35	-2.67
ethane	CC	cyclohexanone	-0.53	-0.36	-2.33	-1.90
pentane	CCCCC	cyclohexanone	-2.70	-2.43		-5.19
2-methylbutane	CCC(C)C	cyclohexanone	-2.58	-2.25		-4.91
2-methylpentane	CCCC(C)C	cyclohexanone	-3.14	-2.94		-6.03
octane	CCCCCCC	cyclohexanone	-4.66	-4.53		-8.70
2,5-dimethylhexane	CC(C)CCC(C)C	cyclohexanone	-4.18	-4.17		-8.05
2,3,4-trimethylpentane	CC(C)(C)C(C)C	cyclohexanone	-4.30	-3.84		-7.57
nonane	CCCCCCCCC	cyclohexanone	-5.25	-5.28	-9.80	-9.87
cyclohexane	C1CCCCC1	cyclohexanone	-3.84	-3.53	-7.12	-6.51
ethene	C=C	cyclohexanone	-0.55	-0.80	-2.28	-2.55
1-pentene	CCCC=C	cyclohexanone	-2.77	-2.80		-5.69
2-methyl-2-butene	CC=C(C)C	cyclohexanone	-3.09	-2.61		-5.31
2-methyl-1,3-butadiene	CC(=C)C=C	cyclohexanone	-3.19	-2.93		-5.77
tetrafluoromethane	FC(F)(F)F	cyclohexanone	1.41	1.10	0.31	-0.07
dichloromethane	ClCCl	cyclohexanone	-4.13	-3.24		-6.23
trichloromethane	ClC(Cl)Cl	cyclohexanone	-4.73	-4.21		-7.97
tetrachloromethane	ClC(Cl)(Cl)Cl	cyclohexanone	-4.32	-4.32		-8.27
1-chloropropane	CCCCl	cyclohexanone	-3.67	-3.26		-6.31
tert-butyl chloride	CC(C)(C)Cl	cyclohexanone	-3.64	-3.45		-6.54
bromoethane	CCBr	cyclohexanone	-3.55	-2.99		-6.03
iodoethane	CCI	cyclohexanone	-4.18	-3.83		-6.97
1,4-dioxane	C1COCCO1	cyclohexanone	-5.00	-4.85	-9.01	-8.67
propanone	CC(C)=O	cyclohexanone	-3.80	-3.36		-6.15
methyl ethyl ketone	CCC(C)=O	cyclohexanone	-4.49	-3.95	-8.24	-7.01
ethanol	CCO	cyclohexanone	-4.31	-4.38		-9.83
nitromethane	C[N+](=O)=O	cyclohexanone	-5.06	-4.51		-8.46
benzene	c1ccccc1	cyclohexanone	-4.50	-4.05	-8.34	-7.39
carbon disulfide	S=C=S	cyclohexanone	-3.31	-2.88		-3.69
acetonitrile	CC#N	cyclohexanone	-4.30	-4.21		-6.62
butane	CCCC	acetophenone	-1.87	-1.86		-4.22
pentane	CCCCC	acetophenone	-2.42	-2.44		-5.11
hexane	CCCCCC	acetophenone	-3.05	-3.04		-6.04
heptane	CCCCCCC	acetophenone	-3.69	-3.58		-6.89

nonane	CCCCCCCCC	acetophenone	-4.88	-4.89		-8.95
2,4-dimethylpentane	CC(C)CC(C)C	acetophenone	-3.14	-3.13		-6.15
cyclohexane	C1CCCCC1	acetophenone	-3.48	-3.32		-6.02
ethylcyclohexane	CCC1CCCCC1	acetophenone	-4.51	-4.48		-7.84
1-pentene	CCCC=C	acetophenone	-2.51	-2.73		-5.38
isopentene	CC(C)C=C	acetophenone	-2.46	-2.63		-5.26
isoprene	CC(=C)C=C	acetophenone	-2.93	-3.03		-5.84
benzene	c1ccccc1	acetophenone	-4.29	-4.33		-7.88
toluene	Cc1ccccc1	acetophenone	-4.97	-4.91		-8.79
1-chloropropane	CCCCl	acetophenone	-3.45	-3.48		-6.70
tetrachloromethane	ClC(Cl)(Cl)Cl	acetophenone	-3.99	-4.44		-8.39
trichloromethane	ClC(Cl)Cl	acetophenone	-4.30	-4.31		-8.03
dichloromethane	ClCCl	acetophenone	-3.79	-3.52		-6.72
bromoethane	CCBr	acetophenone	-3.37	-3.20		-6.42
iodomethane	CI	acetophenone	-3.43	-3.60		-6.82
iodoethane	CCI	acetophenone	-3.99	-4.19		-7.67
methyl ethyl ketone	CCC(C)=O	acetophenone	-4.42	-4.29		-7.69
1,4-dioxane	C1COCCO1	acetophenone	-5.04	-5.12		-9.12
nitromethane	C[N+](=O)[O-]	acetophenone	-4.85	-4.93		-9.39
acetonitrile	CC#N	acetophenone	-4.16	-4.55		-7.32
trimethylamine	CN(C)C	acetophenone	-2.46	-3.12		-6.78
carbon disulfide	S=C=S	acetophenone	-3.20	-2.94		-3.92
methanol	CO	acetophenone	-3.50	-3.89		-8.86
ethanol	CCO	acetophenone	-3.96	-4.41		-9.77
acetophenone	CC(=O)c1ccccc1	acetophenone	-7.64	-7.65		-12.93
acetic acid	CC(O)=O	acetophenone	-6.15	-6.51		-13.34
propanoic acid	CCC(O)=O	acetophenone	-6.71	-6.54		-13.33
hexanoic acid	CCCCC(O)=O	acetophenone	-8.42	-7.65		-15.35
helium	[He]	cyclopentanone	2.38	2.09		2.17
neon	[Ne]	cyclopentanone	2.22	1.95		1.87
argon	[Ar]	cyclopentanone	1.03	0.99		0.27
krypton	[Kr]	cyclopentanone	0.37	0.40		-0.47
xenon	[Xe]	cyclopentanone	-0.47	-0.58		-2.17
hydrogen	[H][H]	cyclopentanone	1.72	1.58		1.13
nitrogen	N#N	cyclopentanone	1.41	0.97		0.38
oxygen	O=O	cyclopentanone	1.10	0.92		-0.12
carbon dioxide	O=C=O	cyclopentanone	-0.89	-0.72		-2.91
tetrafluoromethane	FC(F)(F)F	cyclopentanone	1.36	1.05		-0.06
sulfur hexafluoride	F[S](F)(F)(F)(F)F	cyclopentanone	0.49	0.52		-0.86
methane	C	cyclopentanone	0.69	0.24		-1.04
ethane	CC	cyclopentanone	-0.54	-0.49		-2.07
ethene	C=C	cyclopentanone	-0.60	-0.90		-2.67
cyclohexane	C1CCCCC1	cyclopentanone	-3.74	-3.66		-6.65
benzene	c1ccccc1	cyclopentanone	-4.53	-4.20		-7.62
carbon tetrachloride	ClC(Cl)(Cl)Cl	cyclopentanone	-4.31	-4.47		-8.46
cyclopentanone	O=C1CCCC1	cyclopentanone	-5.82	-5.83		-10.29
dibutyl ether	CCCCOCCCC	cyclopentanone	-5.52	-5.78		-10.23
neon	[Ne]	2-methylcyclohexanone	2.16	1.99		1.97
argon	[Ar]	2-methylcyclohexanone	0.97	0.77		0.20
xenon	[Xe]	2-methylcyclohexanone	-0.56	-0.85		-1.99
hydrogen	[H][H]	2-methylcyclohexanone	1.71	1.35		0.95
deuterium	[H][H]	2-methylcyclohexanone	1.68	1.35		0.95
sulfur hexafluoride	F[S](F)(F)(F)(F)F	2-methylcyclohexanone	0.38	0.33		-0.60
carbon dioxide	O=C=O	2-methylcyclohexanone	-0.71	-0.78		-2.23
ethane	CC	2-methylcyclohexanone	-0.61	-0.89		-2.49
ethene	C=C	2-methylcyclohexanone	-0.58	-1.66		-3.97
carbon tetrafluoride	FC(F)(F)F	2-methylcyclohexanone	1.29	1.00		0.52
2-methylcyclohexanone	CC1CCCC1=O	2-methylcyclohexanone	-6.49	-7.24		-12.54
argon	[Ar]	benzonitrile	1.13	1.10		0.41
carbon monoxide	[C-]#[O+]	benzonitrile	1.08	0.59		-0.56
sulfur dioxide	O=[S]=O	benzonitrile	-2.59	-2.84		-6.90
sulfur hexafluoride	F[S](F)(F)(F)(F)F	benzonitrile	0.71	0.62		-0.58
ethane	CC	benzonitrile	-0.52	-0.64		-2.52
propane	CCC	benzonitrile	-1.11	-1.23		-3.33
butane	CCCC	benzonitrile	-1.81	-1.78		-4.14
pentane	CCCCC	benzonitrile	-2.50	-2.31		-4.91
hexane	CCCCC	benzonitrile	-3.11	-2.85		-5.72
heptane	CCCCC	benzonitrile	-3.74	-3.39		-6.55
octane	CCCCC	benzonitrile	-4.36	-3.91		-7.47
nonane	CCCCC	benzonitrile	-4.97	-4.63		-8.58
2-methylpentane	CCCC(C)C	benzonitrile	-2.89	-2.60		-5.28
2,5-dimethylhexane	CC(C)CCC(C)C	benzonitrile	-3.83	-3.52		-6.75
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	benzonitrile	-3.99	-3.26		-6.42
ethylcyclohexane	CCC1CCCCC1	benzonitrile	-4.55	-4.22		-7.44
ethene	C=C	benzonitrile	-0.45	-0.93		-2.80
isoprene	CC(=C)C=C	benzonitrile	-3.00	-3.02		-5.88
pent-1-ene	CCCC=C	benzonitrile	-2.61	-2.65		-5.28
2-methylbut-2-ene	CC=C(C)C	benzonitrile	-2.89	-2.69		-5.40
hex-1-ene	CCCC=C	benzonitrile	-3.02	-3.27		-6.26
trans-penta-1,3-diene	C/C=C/C=C	benzonitrile	-3.26	-3.09		-5.90
cyclohexene	C1CCC=CC1	benzonitrile	-3.95	-3.89		-7.19
chloromethane	CCl	benzonitrile	-2.19	-2.00		-4.54
dichloromethane	ClCCl	benzonitrile	-3.78	-3.47		-6.68

<i>tert</i> -butyl chloride	CC(C)(C)Cl	benzonitrile	-3.15	-3.56		-6.77
bromoethane	CCBr	benzonitrile	-3.41	-3.08		-6.24
<i>tert</i> -butyl bromide	CC(C)(C)Br	benzonitrile	-3.64	-3.67		-6.97
iodomethane	CI	benzonitrile	-3.41	-3.62		-6.88
iodoethane	CCl	benzonitrile	-4.01	-4.27		-7.87
butanone	CCC(C)=O	benzonitrile	-4.58	-4.32		-7.77
methanol	CO	benzonitrile	-3.38	-3.93		-9.03
ethanol	CCO	benzonitrile	-3.84	-4.45		-9.93
dimethylamine	CNC	benzonitrile	-2.80	-3.44		-7.84
benzene	c1ccccc1	benzonitrile	-4.34	-4.29		-7.85
toluene	Cc1ccccc1	benzonitrile	-5.03	-4.87		-8.75
fluorobenzene	Fc1ccccc1	benzonitrile	-4.53	-4.79		-8.75
chlorobenzene	Clc1ccccc1	benzonitrile	-5.63	-5.77		-10.20
1,2-dichlorobenzene	Clc1ccccc1Cl	benzonitrile	-6.82	-6.84		-11.96
iodobenzene	Ic1ccccc1	benzonitrile	-6.98	-7.10		-11.96
benzonitrile	N#Cc1ccccc1	benzonitrile	-7.31	-8.23		-12.79
benzyl alcohol	OCc1ccccc1	benzonitrile	-8.00	-8.88		-16.76
anthracene	c1ccc2cc3ccccc3cc2c1	benzonitrile	-11.42	-11.07		-18.58
pyrene	c1ccc2ccc3ccccc4ccc(c1)c2c34	benzonitrile	-13.10	-12.78		-21.42
argon	[Ar]	tributyl phosphate	0.97	0.97		0.02
carbon dioxide	O=C=O	tributyl phosphate	-0.68	-1.75		-6.01
nitric oxide	[N]=O	tributyl phosphate	0.80	0.48		-1.02
methane	C	tributyl phosphate	0.44	-0.21		-2.07
ethane	CC	tributyl phosphate	-0.55	-0.99		-3.50
propane	CCC	tributyl phosphate	-1.31	-1.53		-4.46
butane	CCCC	tributyl phosphate	-1.94	-2.09		-5.44
pentane	CCCCC	tributyl phosphate	-2.58	-2.64		-6.39
heptane	CCCCCCC	tributyl phosphate	-3.89	-3.85		-8.34
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	tributyl phosphate	-3.86	-3.73		-8.22
cyclohexane	C1CCCCC1	tributyl phosphate	-3.63	-3.94		-8.29
methylcyclohexane	CC1CCCCC1	tributyl phosphate	-4.02	-4.43		-9.16
ethylcyclohexane	CCC1CCCCC1	tributyl phosphate	-4.71	-5.09		-10.13
propylcyclohexane	CCCC1CCCCC1	tributyl phosphate	-4.80	-5.73		-11.12
<i>cis</i> -1,2-dimethylcyclohexane	C[C@H]1CCCC[C@H]1C	tributyl phosphate	-4.67	-4.96		-9.97
<i>cis</i> -1,4-dimethylcyclohexane	C[C@H]1CC[C@H](C)CC1	tributyl phosphate	-4.56	-4.99		-10.01
ethene	C=C	tributyl phosphate	-0.52	-1.18		-3.96
1-pentene	CCCC=C	tributyl phosphate	-2.62	-2.74		-6.66
1-hexene	CCCCC=C	tributyl phosphate	-3.30	-3.40		-7.64
1-heptene	CCCCC=C	tributyl phosphate	-3.86	-4.05		-8.61
1-octene	CCCCCCC=C	tributyl phosphate	-4.49	-4.71		-9.61
trichloromethane	ClC(Cl)Cl	tributyl phosphate	-4.92	-4.01		-8.24
tetrachloromethane	ClC(Cl)(Cl)Cl	tributyl phosphate	-4.07	-4.39		-8.69
1,2-dichloroethane	ClCCCl	tributyl phosphate	-4.52	-4.29		-9.19
1-chloropropane	CCCCl	tributyl phosphate	-3.42	-3.36		-7.85
1-chlorobutane	CCCCCl	tributyl phosphate	-4.05	-3.94		-8.75
trichloroethene	ClC=C(Cl)Cl	tributyl phosphate	-4.52	-4.21		-8.75
propanone	CC(C)=O	tributyl phosphate	-3.42	-3.65		-8.58
butanone	CCC(C)=O	tributyl phosphate	-4.07	-4.30		-9.48
2-pentanone	CCCC(C)=O	tributyl phosphate	-4.60	-4.95		-10.49
methyl acetate	COC(C)=O	tributyl phosphate	-3.44	-3.86		-8.84
ethyl acetate	CCOC(C)=O	tributyl phosphate	-3.94	-4.29		-9.40
propyl acetate	CCCOC(C)=O	tributyl phosphate	-4.53	-4.89		-10.30
butyl acetate	CCCCOC(C)=O	tributyl phosphate	-5.16	-5.44		-11.08
acetonitrile	CC#N	tributyl phosphate	-3.98	-3.52		-6.83
propionitrile	CCC#N	tributyl phosphate	-4.39	-4.17		-7.82
butyronitrile	CCCC#N	tributyl phosphate	-4.94	-4.69		-8.60
ammonia	N	tributyl phosphate	-1.16	-3.26		-7.62
water	O	tributyl phosphate	-4.22	-4.32		-11.34
methanol	CO	tributyl phosphate	-4.19	-3.02		-7.94
ethanol	CCO	tributyl phosphate	-4.57	-3.46		-8.73
1-propanol	CCCO	tributyl phosphate	-5.32	-4.01		-9.69
hydrogen sulfide	S	tributyl phosphate	-1.73	-1.94		-3.48
benzene	c1ccccc1	tributyl phosphate	-4.15	-4.01		-8.49
toluene	Cc1ccccc1	tributyl phosphate	-4.82	-4.63		-9.44
<i>o</i> -xylene	Cc1ccccc1C	tributyl phosphate	-5.58	-5.21		-10.34
<i>p</i> -xylene	Cc1ccc(C)cc1	tributyl phosphate	-5.42	-5.23		-10.37
isopropylbenzene	CC(C)c1ccccc1	tributyl phosphate	-5.80	-5.90		-11.34
COS	O=C=S	tributyl phosphate	-1.50	-1.67		-3.43
argon	[Ar]	propylene carbonate	1.45	1.35		0.51
hydrogen	[H][H]	propylene carbonate	1.99	1.11		-0.68
nitrogen	N#N	propylene carbonate	1.64	1.77		0.91
carbon dioxide	O=C=O	propylene carbonate	-0.86	-0.57	-3.75	-3.84
hydrogen sulfide	S	propylene carbonate	-1.56	-1.01		-2.34
sulfur dioxide	O=[S]=O	propylene carbonate	-3.25	-3.17	-7.50	-8.89
sulfonyl fluoride	F[S](F)(=O)=O	propylene carbonate	-0.64	-1.18		-3.57
water	O	propylene carbonate	-4.17	-4.11	-8.55	-11.58
ethane	CC	propylene carbonate	-0.14	0.30	-1.37	-1.70
propane	CCC	propylene carbonate	-0.59	-0.30	-1.54	-2.55
pentane	CCCCC	propylene carbonate	-1.66	-1.50	-4.20	-4.40
heptane	CCCCCCC	propylene carbonate	-2.56	-2.63	-5.89	-6.16
octane	CCCCCCCC	propylene carbonate	-3.08	-2.98	-7.51	-6.69
nonane	CCCCCCCCC	propylene carbonate	-3.45	-3.68		-7.82
decane	CCCCCCCCC	propylene carbonate	-4.05	-4.26	-9.08	-8.74

isobutane	CC(C)C	propylene carbonate	-0.87	-0.77	-2.32	-3.26
2-methylpentane	CCCC(C)C	propylene carbonate	-1.98	-1.88		-4.99
2,4-dimethylpentane	CC(C)CC(C)C	propylene carbonate	-2.21	-2.16		-5.43
2,3,4-trimethylpentane	CC(C)(C)C(C)C	propylene carbonate	-2.86	-2.33		-5.76
cyclohexane	C1CCCCC1	propylene carbonate	-2.66	-2.40	-5.78	-5.34
methylcyclopentane	CC1CCCC1	propylene carbonate	-2.41	-2.22	-5.53	-5.03
methylcyclohexane	CC1CCCCC1	propylene carbonate	-2.92	-2.78	-6.27	-5.95
ethylcyclohexane	CCC1CCCCC1	propylene carbonate	-3.41	-3.31		-6.80
ethene	C=C	propylene carbonate	-0.25	-0.43		-3.09
propene	CC=C	propylene carbonate	-0.98	-0.98		-3.81
hex-1-ene	CCCCC=C	propylene carbonate	-2.36	-2.77		-6.51
oct-1-ene	CCCCCCC=C	propylene carbonate	-3.37	-3.76		-8.04
1,3-butadiene	C=CC=C	propylene carbonate	-1.96	-2.14	-4.61	-5.68
cyclohexene	C1CCC=CC1	propylene carbonate	-3.12	-2.87	-6.46	-6.16
benzene	c1ccccc1	propylene carbonate	-3.87	-3.68	-7.72	-7.80
toluene	Cc1ccccc1	propylene carbonate	-4.37	-4.26	-8.52	-8.71
o-xylene	Cc1ccccc1C	propylene carbonate	-5.06	-4.74		-9.49
m-xylene	Cc1ccc(C)c1	propylene carbonate	-4.84	-4.79		-9.54
p-xylene	Cc1ccc(C)cc1	propylene carbonate	-4.83	-4.80		-9.55
diethyl ether	CCOCC	propylene carbonate	-2.58	-2.67	-6.09	-6.07
methyl tert-butyl ether	COC(C)(C)C	propylene carbonate	-3.06	-2.79	-6.95	-6.43
ethyl tert-butyl ether	CCOC(C)(C)C	propylene carbonate	-3.06	-3.23	-7.34	-7.14
methyl tert-pentyl ether	CCC(C)(C)OC	propylene carbonate	-3.53	-3.24		-7.21
isopropyl tert-butyl ether	CC(C)OC(C)(C)C	propylene carbonate	-3.19	-3.48		-7.66
pentan-2-one	CCCC(C)=O	propylene carbonate	-4.75	-4.04		-8.34
dichloromethane	ClCCl	propylene carbonate	-3.48	-2.93	-6.60	-6.84
1,2-dichloroethane	ClCCCl	propylene carbonate	-4.32	-3.98	-7.76	-8.35
t-butyl bromide	CC(C)(C)Br	propylene carbonate	-3.31	-3.34		-7.65
iodoethane	CCl	propylene carbonate	-3.70	-3.47		-7.35
triethylamine	CCN(CC)CC	propylene carbonate	-2.91	-2.99		-7.71
tetramethylstannane	C[Sn](C)(C)C	propylene carbonate	-2.26	-2.38	-5.69	-5.04
helium	[He]	carbon disulfide	2.46	1.93		1.84
neon	[Ne]	carbon disulfide	2.21	1.78		1.54
argon	[Ar]	carbon disulfide	0.96	0.57		-0.18
nitrogen	N#N	carbon disulfide	1.43	0.83		0.46
hydrogen	[H][H]	carbon disulfide	1.62	1.43		1.00
carbon monoxide	[C-]#[O+]	carbon disulfide	1.14	0.29		-0.87
carbon dioxide	O=C=O	carbon disulfide	-0.17	-0.73		-2.73
tetrafluoromethane	FC(F)(F)F	carbon disulfide	1.47	1.08		0.09
sulfur hexafluoride	F[S](F)(F)(F)F	carbon disulfide	0.59	-0.11		-2.08
methane	C	carbon disulfide	0.38	0.01		-1.20
ethane	CC	carbon disulfide	-0.87	-0.85		-2.51
propane	CCC	carbon disulfide	-1.73	-1.67		-3.81
pentane	CCCCC	carbon disulfide	-3.26	-3.22		-6.27
hexane	CCCCCC	carbon disulfide	-4.00	-3.94		-7.40
heptane	CCCCCCC	carbon disulfide	-4.74	-4.65		-8.54
octane	CCCCCCCC	carbon disulfide	-5.47	-5.32		-9.64
nonane	CCCCCCCCC	carbon disulfide	-6.22	-6.06		-10.78
2-methylpentane	CCCC(C)C	carbon disulfide	-3.80	-3.80		-7.17
2,4-dimethylpentane	CC(C)CC(C)C	carbon disulfide	-4.17	-4.35		-8.03
2,5-dimethylhexane	CC(C)CCC(C)C	carbon disulfide	-4.92	-5.07		-9.17
cyclohexane	C1CCCCC1	carbon disulfide	-4.48	-4.41		-7.98
ethylcyclohexane	CCC1CCCCC1	carbon disulfide	-5.65	-5.69		-9.99
trans-2-butene	C/C=C/C	carbon disulfide	-2.86	-2.50		-5.10
1,3-butadiene	C=CC=C	carbon disulfide	-2.72	-2.52		-5.11
ethanol	CCO	carbon disulfide	-2.46	-2.94		-6.15
toluene	Cc1ccccc1	carbon disulfide	-5.27	-5.24		-9.51
1,4-dioxane	C1COCCO1	carbon disulfide	-4.60	-5.38		-9.95
nitromethane	C[N+](=O)=O	carbon disulfide	-3.19	-3.87		-7.69
pentane	CCCCC	triethylamine	-3.28	-3.37	-6.30	-6.76
hexane	CCCCCC	triethylamine	-3.97	-4.07	-7.46	-7.86
heptane	CCCCCCC	triethylamine	-4.68	-4.77	-8.64	-8.93
octane	CCCCCCCC	triethylamine	-5.38	-5.40	-9.81	-9.89
nonane	CCCCCCCCC	triethylamine	-6.07	-6.14	-10.95	-11.07
2-methylpentane	CCCC(C)C	triethylamine	-3.77	-3.99		-7.74
2,4-dimethylpentane	CC(C)CC(C)C	triethylamine	-4.22	-4.56		-8.60
2,5-dimethylhexane	CC(C)CCC(C)C	triethylamine	-4.89	-5.25		-9.67
2,3,4-trimethylpentane	CC(C)(C)C(C)C	triethylamine	-4.99	-5.07		-9.35
ethanol	CCO	triethylamine	-4.17	-3.59	-10.96	-8.10
toluene	Cc1ccccc1	triethylamine	-4.89	-4.97	-8.95	-9.10
1,4-dioxane	C1COCCO1	triethylamine	-4.31	-4.55		-8.43
triethylamine	CCN(CC)CC	triethylamine	-4.50	-4.44	-8.32	-8.28
octane	CCCCCCCC	ethoxybenzene	-4.79	-4.62		-8.21
toluene	Cc1ccccc1	ethoxybenzene	-5.05	-4.90		-8.67
1,4-dioxane	C1COCCO1	ethoxybenzene	-4.85	-4.70		-8.36
octane	CCCCCCCC	2-methylpyridine	-4.82	-4.69		-8.40
methyl ethyl ketone	CCC(C)=O	2-methylpyridine	-4.56	-4.48		-8.00
methanol	CO	2-methylpyridine	-4.47	-3.89		-8.57
1,4-dioxane	C1COCCO1	2-methylpyridine	-5.06	-4.97		-8.50
nitromethane	C[N+](=O)=O	2-methylpyridine	-4.88	-4.92		-9.35
helium	[He]	anisole	2.46	2.14		2.26
neon	[Ne]	anisole	2.31	2.00		1.97
argon	[Ar]	anisole	1.11	0.93		0.29

krypton	[Kr]	anisole	0.44	0.35		-0.37
deuterium	[H][H]	anisole	1.77	1.51		1.07
tetrafluoromethane	FC(F)(F)F	anisole	1.52	1.17		0.34
sulfur hexafluoride	F[S](F)(F)(F)(F)F	anisole	0.62	0.52		-0.98
pentane	CCCCC	anisole	-2.73	-2.54		-4.88
hexane	CCCCCC	anisole	-3.37	-3.32		-6.14
heptane	CCCCCCC	anisole	-4.03	-4.06		-7.35
octane	CCCCCCCC	anisole	-4.68	-4.69		-8.38
2,4-dimethylpentane	CC(C)CC(C)C	anisole	-3.54	-3.86		-7.13
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	anisole	-4.32	-4.46		-8.23
cyclohexane	C1CCCCC1	anisole	-3.80	-3.67		-6.27
methyl ethyl ketone	CCC(C)=O	anisole	-4.49	-4.11		-7.46
ethanol	CCO	anisole	-3.45	-3.91		-8.50
toluene	Cc1ccccc1	anisole	-5.14	-4.95		-8.68
1,4-dioxane	C1COCCO1	anisole	-5.08	-4.76		-8.38
nitromethane	C[N+](=O)=O	anisole	-4.59	-4.61		-9.03
octane	CCCCCCCC	benzyl ether	-4.31	-4.38		-7.87
methyl ethyl ketone	CCC(C)=O	benzyl ether	-4.08	-4.50		-8.78
ethanol	CCO	benzyl ether	-3.28	-3.67		-8.30
toluene	Cc1ccccc1	benzyl ether	-4.82	-4.96		-9.08
1,4-dioxane	C1COCCO1	benzyl ether	-4.77	-5.19		-9.65
octane	CCCCCCCC	3-methylphenol	-4.14	-4.28		-8.43
ethanol	CCO	3-methylphenol	-5.47	-4.37		-10.15
toluene	Cc1ccccc1	3-methylphenol	-4.67	-4.70		-8.76
nitromethane	C[N+](=O)=O	3-methylphenol	-3.24	-4.59		-8.96
hydrogen	[H][H]	acetic acid	1.64	1.35		0.34
argon	[Ar]	acetic acid	0.90	1.21		0.41
krypton	[Kr]	acetic acid	0.52	0.68		-0.36
radon	[Rn]	acetic acid	-0.88	-0.54		-2.51
nitrogen	N#N	acetic acid	1.26	1.12		0.17
ozone	[O-][O+]=O	acetic acid	-0.36	-0.80		-4.09
carbon dioxide	O=C=O	acetic acid	-0.93	-0.45		-3.23
hydrogen sulfide	S	acetic acid	-1.50	-1.52		-2.72
chlorine	ClCl	acetic acid	-2.01	-1.39		-4.18
phosphine	P	acetic acid	-0.69	-0.21		-1.64
methane	C	acetic acid	0.52	0.57		-0.93
ethane	CC	acetic acid	-0.38	-0.17		-1.95
propane	CCC	acetic acid	-0.95	-0.86		-2.97
butane	CCCC	acetic acid	-1.21	-1.62		-4.17
2-methylpropane	CC(C)C	acetic acid	-1.31	-1.47		-3.92
pentane	CCCCC	acetic acid	-2.06	-2.35	-5.20	-5.31
hexane	CCCCCC	acetic acid	-2.67	-3.09	-6.19	-6.50
heptane	CCCCCCC	acetic acid	-3.19	-3.79	-7.25	-7.61
cyclopentane	C1CCCC1	acetic acid	-2.62	-2.77	-5.65	-5.55
cyclohexane	C1CCCCC1	acetic acid	-3.22	-3.50	-6.55	-6.74
ethene	C=C	acetic acid	-0.75	-0.56		-2.62
propene	CC=C	acetic acid	-1.34	-1.19		-3.52
trans-2-butene	C/C=C/C	acetic acid	-2.28	-1.85		-4.49
1,3-butadiene	C=CC=C	acetic acid	-2.44	-2.01		-4.66
ethanol	CCO	acetic acid	-5.20	-3.90	-9.26	-9.24
1,4-dioxane	C1COCCO1	acetic acid	-5.86	-4.61	-9.52	-8.72
butanone	CCC(C)=O	acetic acid	-4.89	-3.87		-7.52
acetonitrile	CC#N	acetic acid	-4.01	-3.41		-5.69
benzene	c1ccccc1	acetic acid	-3.85	-4.15	-7.65	-8.14
toluene	Cc1ccccc1	acetic acid	-4.58	-4.86	-8.74	-9.25
fluoroethane	CCF	acetic acid	-1.41	-1.24		-3.54
2-bromo-2-methylpropane	CC(C)(C)Br	acetic acid	-3.43	-3.56	-7.11	-7.28
octane	CCCCCCCC	nitroethane	-4.02	-3.65		-6.62
ethanol	CCO	nitroethane	-3.85	-3.89		-8.66
toluene	Cc1ccccc1	nitroethane	-4.97	-4.56		-8.06
1,4-dioxane	C1COCCO1	nitroethane	-5.32	-4.50		-7.70
pentane	CCCCC	benzyl alcohol	-2.11	-2.24		-5.08
hexane	CCCCCC	benzyl alcohol	-2.68	-2.85		-6.05
heptane	CCCCCCC	benzyl alcohol	-3.23	-3.58		-7.26
octane	CCCCCCCC	benzyl alcohol	-3.80	-4.22		-8.36
nonane	CCCCCCCCC	benzyl alcohol	-4.36	-5.02		-9.64
2-methylpentane	CCCC(C)C	benzyl alcohol	-2.48	-2.70		-5.85
2,5-dimethylhexane	CC(C)CCC(C)C	benzyl alcohol	-3.32	-3.92		-7.82
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	benzyl alcohol	-3.54	-3.69		-7.56
cyclohexane	C1CCCCC1	benzyl alcohol	-3.22	-3.51		-6.89
ethylcyclohexane	CCC1CCCCC1	benzyl alcohol	-4.14	-4.69		-8.75
methyl ethyl ketone	CCC(C)=O	benzyl alcohol	-4.65	-4.18		-7.90
ethanol	CCO	benzyl alcohol	-4.73	-4.38		-10.20
1,4-dioxane	C1COCCO1	benzyl alcohol	-5.47	-5.20		-9.84
nitromethane	C[N+](=O)=O	benzyl alcohol	-4.47	-4.62		-9.03
pentane	CCCCC	butyronitrile	-2.62	-2.39		-5.30
heptane	CCCCCCC	butyronitrile	-3.79	-3.80		-7.59
2,4-dimethylpentane	CC(C)CC(C)C	butyronitrile	-3.38	-3.38		-6.90
octane	CCCCCCCC	butyronitrile	-4.38	-4.49		-8.79
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	butyronitrile	-4.10	-3.77		-7.60
nonane	CCCCCCCCC	butyronitrile	-4.98	-5.22		-9.91
cyclohexane	C1CCCCC1	butyronitrile	-3.64	-3.69		-7.09
methylcyclohexane	CC1CCCCC1	butyronitrile	-4.08	-4.21		-7.92



ethylcyclohexane	CCC1CCCCC1	butyronitrile	-4.55	-4.92		-9.08
1-heptene	CCCCC=C	butyronitrile	-3.92	-4.07		-7.91
hepta-1,6-diene	C=CCCCC=C	butyronitrile	-4.06	-4.49		-8.47
benzene	c1ccccc1	butyronitrile	-4.41	-3.96		-7.36
toluene	Cc1ccccc1	butyronitrile	-5.04	-4.63		-8.46
ethylbenzene	CCc1ccccc1	butyronitrile	-5.66	-5.36		-9.60
methanol	CO	butyronitrile	-3.65	-3.68		-8.60
ethanol	CCO	butyronitrile	-4.10	-4.25		-9.66
propan-1-ol	CCCO	butyronitrile	-4.73	-4.92		-10.78
propan-2-ol	CC(C)O	butyronitrile	-4.31	-4.64		-10.28
butan-2-ol	CCC(C)O	butyronitrile	-4.93	-5.34		-11.55
pentan-1-ol	CCCCCO	butyronitrile	-6.06	-6.31		-13.15
hexan-1-ol	CCCCCO	butyronitrile	-6.65	-6.88		-14.08
nonan-1-ol	CCCCCCCCCO	butyronitrile	-8.43	-8.96		-17.28
decan-1-ol	CCCCCCCCCO	butyronitrile	-8.93	-9.53		-18.28
propionitrile	CCC#N	butyronitrile	-4.98	-4.73		-7.56
butyronitrile	CCCC#N	butyronitrile	-5.49	-5.30		-8.54
butanone	CCC(C)=O	butyronitrile	-4.63	-3.83		-6.88
1,4-dioxane	C1COCCO1	butyronitrile	-5.05	-4.72		-8.54
nitromethane	C[N+](=O)=O	butyronitrile	-5.07	-4.27		-8.04
hydrogen	[H][H]	aniline	2.11	1.59		0.93
xenon	[Xe]	aniline	0.38	-0.31		-2.16
radon	[Rn]	aniline	-0.74	-0.61		-2.62
oxygen	O=O	aniline	1.66	0.70		-1.17
carbon dioxide	O=C=O	aniline	-0.17	-0.54		-3.25
methane	C	aniline	1.05	0.19		-1.64
ethane	CC	aniline	-0.23	-0.53		-2.63
propane	CCC	aniline	-0.79	-1.12		-3.45
butane	CCCC	aniline	-1.40	-1.73		-4.37
2-methylpropane	CC(C)C	aniline	-1.07	-1.68		-4.35
pentane	CCCCC	aniline	-1.81	-2.32		-5.28
2-methylbutane	CCC(C)C	aniline	-1.54	-2.26		-5.25
hexane	CCCCCC	aniline	-2.33	-3.06		-6.48
heptane	CCCCCCC	aniline	-2.98	-3.82		-7.72
octane	CCCCCCCC	aniline	-3.53	-4.46		-8.81
cyclopentane	C1CCCC1	aniline	-2.55	-3.09		-6.36
cyclohexane	C1CCCCC1	aniline	-3.01	-3.72		-7.33
methylcyclohexane	CC1CCCCC1	aniline	-3.31	-4.30		-8.27
ethylcyclohexane	CCC1CCCCC1	aniline	-3.89	-5.00		-9.38
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	aniline	-2.81	-3.81		-7.88
ethene	C=C	aniline	-0.15	-0.78		-2.92
propene	CC=C	aniline	-1.08	-1.45		-3.93
1-hexene	CCCCC=C	aniline	-2.67	-3.26		-6.69
1-octene	CCCCC=C	aniline	-3.81	-4.75		-9.14
2-methyl-1-butene	CCC(C)=C	aniline	-1.99	-2.64		-5.79
2-methyl-1-pentene	CCCC(C)=C	aniline	-2.68	-3.23		-6.70
cyclohexene	C1CCC=CC1	aniline	-3.49	-3.98		-7.79
1,3-butadiene	C=CC=C	aniline	-2.06	-2.38		-5.31
dichloromethane	ClCCl	aniline	-3.44	-3.28		-6.77
tetrachloromethane	ClC(Cl)(Cl)Cl	aniline	-3.52	-4.49		-8.98
1-chloropropane	CCCCl	aniline	-3.14	-3.12		-6.42
1-chlorobutane	CCCCCl	aniline	-3.83	-3.87		-7.65
2-chloro-2-methylpropane	CC(C)(C)Cl	aniline	-2.93	-3.39		-6.83
ethyl bromide	CCBr	aniline	-3.14	-2.88		-6.21
ethyl iodide	CCI	aniline	-3.72	-3.93		-7.66
diethyl ether	CCOCC	aniline	-3.77	-3.39		-6.93
1,4-dioxane	C1COCCO1	aniline	-5.67	-5.10		-9.82
ethyl acetate	CCOC(C)=O	aniline	-4.34	-4.24		-8.22
propanone	CC(C)=O	aniline	-4.13	-3.46		-6.92
methyl ethyl ketone	CCC(C)=O	aniline	-4.87	-4.06		-7.79
nitromethane	C[N+](=O)=O	aniline	-5.03	-4.45		-8.89
methanol	CO	aniline	-3.86	-3.54		-8.67
ethanol	CCO	aniline	-4.30	-4.14		-9.75
1-butanol	CCCCO	aniline	-5.38	-5.54		-12.10
benzene	c1ccccc1	aniline	-4.08	-4.05		-7.87
toluene	Cc1ccccc1	aniline	-4.64	-4.81		-9.11
1,2-dimethylbenzene	Cc1ccccc1C	aniline	-5.40	-5.52		-10.29
chlorobenzene	Clc1ccccc1	aniline	-5.16	-5.49		-10.12
aniline	Nc1ccccc1	aniline	-7.47	-8.07		-15.08
chlorodifluoromethane	FC(F)Cl	nitromethane	-1.80	-1.56		-3.42
pentane	CCCCC	nitromethane	-1.81	-1.89	-3.54	-3.83
hexane	CCCCC	nitromethane	-2.26	-2.48	-4.27	-4.76
heptane	CCCCC	nitromethane	-2.69	-3.02	-4.96	-5.60
octane	CCCCC	nitromethane	-3.13	-3.46	-6.50	-6.29
nonane	CCCCC	nitromethane	-3.58	-4.32		-7.71
2,4-dimethylpentane	CC(C)CC(C)C	nitromethane	-2.39	-2.56		-4.88
2,5-dimethylhexane	CC(C)CCC(C)C	nitromethane	-2.83	-3.27		-6.04
2,3,4-trimethylpentane	CC(C)(C)C(C)C	nitromethane	-3.01	-2.98		-5.64
ethylcyclohexane	CCC1CCCCC1	nitromethane	-3.46	-3.97		-6.72
methyl ethyl ketone	CCC(C)=O	nitromethane	-4.77	-4.29		-7.87
toluene	Cc1ccccc1	nitromethane	-4.60	-4.64	-7.86	-8.18
1-chlorobutane	CCCCl	nitromethane	-3.70	-3.91	-6.42	-7.30
ethyl acetate	CCOC(C)=O	nitromethane	-4.57	-4.56		-8.27

acetonitrile	CC#N	nitromethane	-4.84	-4.29	-7.87	-6.78
triethylamine	CCN(CC)CC	nitromethane	-3.58	-3.61		-7.55
helium	[He]	nitrobenzene	2.79	2.24		2.30
neon	[Ne]	nitrobenzene	2.61	2.12		2.15
argon	[Ar]	nitrobenzene	1.33	1.22		0.70
krypton	[Kr]	nitrobenzene	0.64	0.75		0.14
hydrogen	[H][H]	nitrobenzene	3.31	1.53		0.89
oxygen	O=O	nitrobenzene	1.27	-0.17		-2.63
pentane	CCCCC	nitrobenzene	-2.36	-2.16		-4.41
heptane	CCCCCCC	nitrobenzene	-3.58	-3.16		-5.86
octane	CCCCCCCC	nitrobenzene	-4.19	-3.48		-6.26
2-methylpentane	CCCC(C)C	nitrobenzene	-2.75	-2.51		-4.91
2,4-dimethylpentane	CC(C)CC(C)C	nitrobenzene	-3.09	-2.77		-5.25
2,5-dimethylhexane	CC(C)CCC(C)C	nitrobenzene	-3.68	-3.26		-5.97
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	nitrobenzene	-3.86	-2.98		-5.66
cyclohexane	C1CCCCC1	nitrobenzene	-3.39	-3.10		-5.55
ethylcyclohexane	CCC1CCCCC1	nitrobenzene	-4.43	-3.89		-6.65
methyl ethyl ketone	CCC(C)=O	nitrobenzene	-4.48	-4.66		-8.86
ethanol	CCO	nitrobenzene	-3.44	-3.99		-8.93
toluene	Cc1ccccc1	nitrobenzene	-4.99	-5.14		-9.38
1,4-dioxane	C1COCCO1	nitrobenzene	-5.15	-5.08		-9.00
nitromethane	C[N+](=O)[O-]	nitrobenzene	-4.84	-5.69		-11.39
helium	[He]	dimethyl sulfoxide	2.74	1.84		1.55
xenon	[Xe]	dimethyl sulfoxide	0.32	0.15		-2.11
deuterium	[H][H]	dimethyl sulfoxide	2.13	1.67		1.00
nitrogen	N#N	dimethyl sulfoxide	2.11	1.19		-0.75
oxygen	O=O	dimethyl sulfoxide	1.73	0.89		-1.14
carbon dioxide	O=C=O	dimethyl sulfoxide	-0.67	-0.26	-2.97	-3.48
methane	C	dimethyl sulfoxide	1.20	1.05		-0.67
ethane	CC	dimethyl sulfoxide	0.29	0.66		-1.32
hexane	CCCCCC	dimethyl sulfoxide	-1.91	-1.85	-4.21	-5.18
heptane	CCCCCCC	dimethyl sulfoxide	-2.35	-2.41	-5.05	-6.07
octane	CCCCCCCC	dimethyl sulfoxide	-2.78	-2.89	-5.76	-6.92
nonane	CCCCCCCCC	dimethyl sulfoxide	-3.22	-3.47	-6.61	-7.78
2,4-dimethylpentane	CC(C)CC(C)C	dimethyl sulfoxide	-1.97	-1.88		-5.21
2,5-dimethylhexane	CC(C)CCC(C)C	dimethyl sulfoxide	-2.38	-2.46		-6.13
cyclopentane	C1CCCC1	dimethyl sulfoxide	-1.98	-1.91		-5.13
methylcyclopentane	CC1CCCC1	dimethyl sulfoxide	-2.20	-2.37		-5.85
cyclohexane	C1CCCCC1	dimethyl sulfoxide	-2.56	-2.51	-5.16	-6.08
methylcyclohexane	CC1CCCCC1	dimethyl sulfoxide	-2.68	-2.88		-6.65
ethylcyclohexane	CCC1CCCCC1	dimethyl sulfoxide	-3.26	-3.44		-7.55
ethene	C=C	dimethyl sulfoxide	-0.05	0.13		-2.23
methyl ethyl ketone	CCC(C)=O	dimethyl sulfoxide	-4.29	-3.48	-7.76	-7.57
methanol	CO	dimethyl sulfoxide	-5.10	-3.10	-9.36	-8.82
ethanol	CCO	dimethyl sulfoxide	-5.34	-3.63	-9.83	-9.77
1-propanol	CCCO	dimethyl sulfoxide	-5.69	-4.18	-10.46	-10.66
isopropanol	CC(C)O	dimethyl sulfoxide	-5.11	-3.84	-9.93	-10.17
toluene	Cc1ccccc1	dimethyl sulfoxide	-4.52	-3.88	-8.22	-8.23
diethyl ether	CCOCC	dimethyl sulfoxide	-2.30	-2.36	-5.16	-5.78
diisopropyl ether	CC(C)OC(C)C	dimethyl sulfoxide	-2.51	-3.23	-6.34	-7.40
methyl <i>tert</i> -butyl ether	COC(C)(C)C	dimethyl sulfoxide	-2.64	-2.52	-5.79	-6.22
methyl <i>tert</i> -amyl ether	CCC(C)(C)OC	dimethyl sulfoxide	-3.14	-3.03	-6.95	-7.14
tetrahydrofuran	C1CCOC1	dimethyl sulfoxide	-3.65	-3.18	-6.53	-7.16
1,4-dioxane	C1COCCO1	dimethyl sulfoxide	-4.96	-4.25	-8.75	-8.95
nitromethane	C[N+](=O)[O-]	dimethyl sulfoxide	-5.59	-4.24	-9.31	-9.28
carbon monoxide	[C-]#[O+]	propionitrile	0.90	0.67		-0.36
carbon dioxide	O=C=O	propionitrile	-1.05	-0.80		-3.05
pentane	CCCCC	propionitrile	-2.43	-2.34		-5.03
hexane	CCCCCC	propionitrile	-3.00	-2.92		-5.94
2-methylpentane	CCCC(C)C	propionitrile	-2.83	-2.70		-5.58
heptane	CCCCCCC	propionitrile	-3.52	-3.60		-7.06
2,4-dimethylpentane	CC(C)CC(C)C	propionitrile	-3.17	-3.17		-6.37
octane	CCCCCCCC	propionitrile	-4.13	-4.28		-8.26
2,5-dimethylhexane	CC(C)CCC(C)C	propionitrile	-3.76	-3.90		-7.55
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	propionitrile	-3.86	-3.56		-7.06
cyclohexane	C1CCCCC1	propionitrile	-3.42	-3.48		-6.53
1-pentene	CCCC=C	propionitrile	-2.67	-2.77		-5.64
1-heptene	CCCCC=C	propionitrile	-3.79	-3.93		-7.48
isopentene	CC(C)C=C	propionitrile	-2.47	-2.60		-5.38
hepta-1,6-diene	C=CCCC=C	propionitrile	-3.97	-4.47		-8.28
isoprene	CC(=C)C=C	propionitrile	-3.09	-2.97		-5.88
benzene	c1ccccc1	propionitrile	-4.33	-4.10		-7.51
trichloromethane	ClC(Cl)Cl	propionitrile	-4.33	-4.17		-7.91
1-chloropropane	CCCCl	propionitrile	-3.56	-3.27		-6.34
<i>tert</i> -butyl chloride	CC(C)(C)Cl	propionitrile	-3.51	-3.29		-6.20
bromoethane	CCBr	propionitrile	-3.42	-2.91		-5.88
iodomethane	CI	propionitrile	-3.38	-3.18		-5.89
iodoethane	CCl	propionitrile	-3.90	-3.75		-6.71
methanol	CO	propionitrile	-3.68	-3.73		-8.53
ethanol	CCO	propionitrile	-4.05	-4.30		-9.58
propan-1-ol	CCCO	propionitrile	-4.65	-4.89		-10.58
propan-2-ol	CC(C)O	propionitrile	-4.19	-4.69		-10.24
butan-1-ol	CCCCO	propionitrile	-5.27	-5.40		-11.42

acetonitrile	CC#N	propionitrile	-4.69	-4.34		-6.85
propionitrile	CCC#N	propionitrile	-5.13	-4.94		-7.83
butyronitrile	CCCC#N	propionitrile	-5.62	-5.53		-8.85
butanone	CCC(C)=O	propionitrile	-4.68	-4.04		-7.14
carbon disulfide	S=C=S	propionitrile	-2.89	-2.55		-3.14
ethyl acetate	CCOC(C)=O	propionitrile	-4.48	-4.29		-7.56
pyridine	c1ccncc1	propionitrile	-5.44	-5.64		-9.29
hydrogen	[H][H]	acetonitrile	1.45	1.62	1.56	1.20
hydrogen sulfide	S	acetonitrile	-1.86	-1.91		-3.49
nitric oxide	[N]=O	acetonitrile	0.66	0.55	-0.44	-0.50
2-methylpropane	CC(C)C	acetonitrile	-1.40	-1.44		-3.50
pentane	CCCCC	acetonitrile	-2.19	-2.22	-4.25	-4.73
hexane	CCCCCC	acetonitrile	-2.62	-2.80	-5.13	-5.64
heptane	CCCCCCC	acetonitrile	-3.12	-3.37	-5.85	-6.57
octane	CCCCCCCC	acetonitrile	-3.61	-3.99	-6.74	-7.66
nonane	CCCCCCCCC	acetonitrile	-4.12	-4.67		-8.67
2-methylpentane	CCCC(C)C	acetonitrile	-2.48	-2.57	-4.77	-5.27
3-methylpentane	CCC(C)CC	acetonitrile	-2.46	-2.53		-5.21
2-methylhexane	CCCCC(C)C	acetonitrile	-3.07	-3.12		-6.14
2,3-dimethylpentane	CCC(C)C(C)C	acetonitrile	-3.20	-2.88		-5.82
2,4-dimethylpentane	CC(C)CC(C)C	acetonitrile	-2.77	-2.87		-5.76
2,5-dimethylhexane	CC(C)CCC(C)C	acetonitrile	-3.26	-3.56		-6.86
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	acetonitrile	-3.19	-3.32	-6.22	-6.77
cyclopentane	C1CCCC1	acetonitrile	-2.52	-2.64		-5.07
methylcyclopentane	CC1CCCC1	acetonitrile	-2.80	-3.00		-5.60
cyclohexane	C1CCCCC1	acetonitrile	-3.01	-3.25	-5.56	-6.07
ethylcyclohexane	CCC1CCCCC1	acetonitrile	-3.84	-4.34		-7.78
isobutylene	CC(C)=C	acetonitrile	-2.04	-2.06		-4.51
1-pentene	CCCC=C	acetonitrile	-2.41	-2.66		-5.34
1-heptene	CCCCCC=C	acetonitrile	-3.35	-3.78		-7.11
cyclohexene	C1CCC=CC1	acetonitrile	-3.43	-3.79		-7.02
acetone	CC(C)=O	acetonitrile	-4.32	-3.56	-7.86	-6.46
methyl ethyl ketone	CCC(C)=O	acetonitrile	-4.78	-4.18	-8.32	-7.39
ethanol	CCO	acetonitrile	-4.34	-4.27	-8.23	-9.45
toluene	Cc1ccccc1	acetonitrile	-4.73	-4.76	-8.92	-8.55
1,4-dioxane	C1COCCO1	acetonitrile	-5.24	-4.94		-8.78
chloroform	ClC(Cl)Cl	acetonitrile	-4.29	-4.17	-7.78	-7.85
carbon tetrachloride	ClC(Cl)(Cl)Cl	acetonitrile	-3.66	-4.17		-7.91
1-chlorobutane	CCCCCl	acetonitrile	-3.93	-3.90	-7.17	-7.28
2-chloro-2-methylpropane	CC(C)(C)Cl	acetonitrile	-3.33	-3.25	-6.20	-6.09
bromoethane	CCBr	acetonitrile	-3.29	-2.81		-5.63
iodomethane	CI	acetonitrile	-3.21	-3.33		-6.13
iodoethane	CCI	acetonitrile	-3.69	-3.87		-6.90
acetonitrile	CC#N	acetonitrile	-4.89	-4.44	-7.87	-7.00
triethylamine	CCN(CC)CC	acetonitrile	-3.67	-4.02	-7.05	-8.63
pentane	CCCCC	ethyl benzoate	-2.65	-2.45		-5.01
hexane	CCCCCC	ethyl benzoate	-3.31	-3.16		-6.13
heptane	CCCCCCC	ethyl benzoate	-3.99	-3.84		-7.15
1-pentene	CCCC=C	ethyl benzoate	-2.73	-2.99		-6.03
1-hexene	CCCCC=C	ethyl benzoate	-3.88	-3.53		-6.79
1-octene	CCCCCCC=C	ethyl benzoate	-4.75	-4.82		-8.71
cyclopentane	C1CCCC1	ethyl benzoate	-3.16	-2.96		-5.56
cyclohexane	C1CCCCC1	ethyl benzoate	-3.75	-3.66		-6.65
methylcyclopentane	CC1CCCC1	ethyl benzoate	-3.56	-3.57		-6.52
cyclohexene	C1CCC=CC1	ethyl benzoate	-4.04	-3.87		-7.03
benzene	c1ccccc1	ethyl benzoate	-4.30	-4.22		-7.86
toluene	Cc1ccccc1	ethyl benzoate	-4.96	-4.97		-9.09
ethylbenzene	CCc1ccccc1	ethyl benzoate	-5.55	-5.60		-9.99
<i>o</i> -xylene	Cc1ccccc1C	ethyl benzoate	-5.82	-5.63		-10.15
<i>m</i> -xylene	Cc1ccc(C)c1	ethyl benzoate	-5.68	-5.67		-10.23
<i>p</i> -xylene	Cc1ccc(C)cc1	ethyl benzoate	-5.64	-5.67		-10.23
diisopropyl ether	CC(C)OC(C)C	ethyl benzoate	-3.69	-4.14		-7.65
methyl <i>tert</i> -butyl ether	COC(C)(C)C	ethyl benzoate	-3.53	-3.55		-6.82
ethyl <i>tert</i> -butyl ether	CCOC(C)(C)C	ethyl benzoate	-3.85	-4.01		-7.51
methyl <i>tert</i> -pentyl ether	CCC(C)(C)OC	ethyl benzoate	-4.23	-3.95		-7.37
carbon dioxide	O=C=O	sulfolane	-0.65	0.22		-3.15
sulfur dioxide	O=[S]=O	sulfolane	-3.29	-2.72		-8.67
hydrogen sulfide	S	sulfolane	-1.60	-1.58		-4.62
pentane	CCCCC	sulfolane	-1.39	-1.35		-5.10
hexane	CCCCCC	sulfolane	-1.93	-1.96		-6.06
octane	CCCCCCCC	sulfolane	-2.73	-2.92		-7.61
nonane	CCCCCCCCC	sulfolane	-3.19	-3.63		-8.76
decane	CCCCCCCCC	sulfolane	-3.70	-4.35		-9.92
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	sulfolane	-2.33	-2.15		-6.44
cyclohexane	C1CCCCC1	sulfolane	-2.46	-2.75		-7.29
cycloheptane	C1CCCCC1	sulfolane	-3.14	-3.29		-8.12
cyclooctane	C1CCCCC1	sulfolane	-3.81	-3.79		-8.94
methylcyclopentane	CC1CCCC1	sulfolane	-2.21	-2.60		-7.07
1-butene	CCC=C	sulfolane	-1.23	-1.22		-4.90
<i>trans</i> -2-butene	C/C=C/C	sulfolane	-1.35	-1.26		-4.97
<i>cis</i> -2-butene	C/C=C/C	sulfolane	-1.48	-1.26		-4.95
1-heptene	CCCCCC=C	sulfolane	-2.59	-2.87		-7.37
1-octene	CCCCCCC=C	sulfolane	-3.07	-3.40		-8.15

cyclohexene	C1CCCC=CC1	sulfolane	-3.00	-2.91		-7.32
1-hexyne	CCCCC#C	sulfolane	-3.28	-2.87		-7.43
1-heptyne	CCCCC#C	sulfolane	-3.91	-3.32		-8.02
1-octyne	CCCCC#C	sulfolane	-4.21	-3.76		-8.65
dichloromethane	ClCCl	sulfolane	-3.69	-2.65		-7.28
chloroform	ClC(Cl)Cl	sulfolane	-4.14	-3.40		-8.51
carbon tetrachloride	ClC(Cl)(Cl)Cl	sulfolane	-3.50	-3.56		-8.94
1,2-dichloroethane	ClCCCl	sulfolane	-4.56	-3.61		-8.55
trichloroethene	ClC=C(Cl)Cl	sulfolane	-3.96	-3.73		-9.13
acetonitrile	CC#N	sulfolane	-4.51	-3.66		-7.62
diisopropyl ether	CC(C)OC(C)C	sulfolane	-2.65	-3.36		-8.34
methyl <i>tert</i> -butyl ether	COC(C)(C)C	sulfolane	-2.76	-2.81		-7.54
ethyl <i>tert</i> -butyl ether	CCOC(C)(C)C	sulfolane	-2.83	-3.27		-8.30
methyl <i>tert</i> -amyl ether	CCC(C)(C)OC	sulfolane	-3.30	-3.26		-8.30
methyl formate	COC=O	sulfolane	-3.23	-2.78		-7.17
methyl acetate	COC(C)=O	sulfolane	-3.64	-3.14		-7.55
ethyl acetate	CCOC(C)=O	sulfolane	-3.92	-3.40		-7.98
propyl acetate	CCCOC(C)=O	sulfolane	-4.33	-3.81		-8.73
butyl acetate	CCCCOC(C)=O	sulfolane	-4.82	-4.21		-9.41
acetaldehyde	CC=O	sulfolane	-2.92	-2.08		-6.13
isobutyraldehyde	CC(C)C=O	sulfolane	-3.64	-3.31		-8.08
butanone	CCC(C)=O	sulfolane	-4.13	-3.36		-8.08
methyl isobutyl ketone	CC(C)CC(C)=O	sulfolane	-4.67	-4.28		-9.62
isopropanol	CC(C)O	sulfolane	-4.04	-3.91		-11.12
isobutanol	CC(C)CO	sulfolane	-4.88	-4.65		-12.22
nitromethane	C[N+](=O)[O-]	sulfolane	-5.28	-3.82		-9.17
toluene	Cc1ccccc1	sulfolane	-4.46	-3.84		-8.76
ethylbenzene	CCc1ccccc1	sulfolane	-4.87	-4.41		-9.58
<i>o</i> -xylene	Cc1ccccc1C	sulfolane	-5.10	-4.33		-9.53
<i>p</i> -xylene	Cc1ccc(C)cc1	sulfolane	-4.81	-4.39		-9.59
chlorobenzene	Clc1ccccc1	sulfolane	-5.14	-4.76		-10.24
pyridine	c1ccncc1	sulfolane	-5.22	-5.22		-10.63
hydrogen	[H][H]	pyridine	1.79	1.53		1.12
oxygen	O=O	pyridine	1.17	0.71		-0.18
nitrous oxide	[O-][N+]=[N]	pyridine	-0.72	-1.20		-2.66
carbon monoxide	[C-]#[O+]	pyridine	1.27	0.37		-0.60
carbon dioxide	O=C=O	pyridine	-0.76	-0.97		-3.04
methane	C	pyridine	0.64	0.04		-1.02
pentane	CCCCC	pyridine	-2.62	-2.61		-5.02
hexane	CCCCCC	pyridine	-3.23	-3.32		-6.18
heptane	CCCCCCC	pyridine	-3.86	-4.04		-7.34
nonane	CCCCCCCC	pyridine	-5.09	-5.41		-9.55
decane	CCCCCCCCC	pyridine	-5.76	-6.13		-10.70
undecane	CCCCCCCCC	pyridine	-6.46	-6.67		-11.59
2-methylpentane	CCCC(C)C	pyridine	-3.02	-3.17		-5.96
2,4-dimethylpentane	CC(C)CC(C)C	pyridine	-3.37	-3.69		-6.84
2,5-dimethylhexane	CC(C)CCC(C)C	pyridine	-4.04	-4.40		-7.98
2,3,4-trimethylpentane	CC(C)(C)C(C)C	pyridine	-4.14	-4.15		-7.67
1-pentene	CCCC=C	pyridine	-2.70	-3.08		-5.76
1-heptene	CCCCC=C	pyridine	-4.14	-4.41		-7.96
cyclohexene	C1CCCC=CC1	pyridine	-4.12	-4.03		-6.92
1-heptyne	CCCCC#C	pyridine	-4.71	-4.78		-8.41
1,2-dichloropropane	CC(Cl)CCl	pyridine	-5.00	-5.27		-9.00
isopropylbromide	CC(C)Br	pyridine	-3.95	-3.75		-6.82
1,4-dioxane	C1COCCO1	pyridine	-5.20	-5.07	-9.42	-8.58
acetone	CC(C)=O	pyridine	-3.99	-4.08	-7.34	-7.41
methyl isobutyl ketone	CC(C)CC(C)=O	pyridine	-5.53	-5.59		-9.65
2-octanone	CCCCC(C)=O	pyridine	-7.12	-7.18	-12.26	-12.16
butyl acetate	CCCCOC(C)=O	pyridine	-5.79	-5.75		-9.94
pentyl acetate	CCCCCOC(C)=O	pyridine	-6.43	-6.41		-11.05
acetonitrile	CC#N	pyridine	-4.43	-4.80		-7.69
nitromethane	C[N+](=O)[O-]	pyridine	-5.04	-5.12		-9.62
methanol	CO	pyridine	-4.61	-3.95	-9.54	-8.57
ethanol	CCO	pyridine	-5.02	-4.44	-9.97	-9.37
1-propanol	CCCO	pyridine	-5.59	-5.01		-10.25
isopropanol	CC(C)O	pyridine	-4.96	-4.69		-9.79
1-butanol	CCCCO	pyridine	-6.22	-5.68		-11.39
2-butanol	CCC(C)O	pyridine	-5.64	-5.25		-10.58
isobutanol	CC(C)CO	pyridine	-6.02	-5.59		-11.25
benzene	c1ccccc1	pyridine	-4.51	-4.51	-8.37	-7.88
ethylbenzene	CCc1ccccc1	pyridine	-5.76	-5.93		-10.17
<i>o</i> -xylene	Cc1ccccc1C	pyridine	-5.99	-5.90		-10.19
<i>m</i> -xylene	Cc1ccc(C)cc1	pyridine	-5.81	-5.95		-10.29
<i>p</i> -xylene	Cc1ccc(C)cc1	pyridine	-5.76	-5.95		-10.30
fluorobenzene	Fc1ccccc1	pyridine	-4.69	-4.94	-8.25	-8.69
chlorobenzene	Clc1ccccc1	pyridine	-5.82	-5.92	-9.58	-10.14
1,2-dichlorobenzene	Clc1ccccc1Cl	pyridine	-7.06	-7.05	-11.74	-11.99
pyridine	c1ccncc1	pyridine	-5.52	-6.12	-9.61	-10.01
water	O	pyridine	-4.17	-4.15	-10.99	-9.70
helium	[He]	dimethyl carbonate	2.10	2.39		2.80
neon	[Ne]	dimethyl carbonate	1.96	2.23	3.66	2.46
argon	[Ar]	dimethyl carbonate	0.86	1.20	1.82	0.78
krypton	[Kr]	dimethyl carbonate	0.30	0.43	-0.60	-0.26

xenon	[Xe]	dimethyl carbonate	-0.44	-0.25	-1.35	-1.18
hydrogen	[H][H]	dimethyl carbonate	1.58	0.68		-0.24
nitrogen	N#N	dimethyl carbonate	1.15	1.48		1.44
sulfur hexafluoride	F[S](F)(F)(F)(F)F	dimethyl carbonate	0.10	0.45	-0.80	-0.44
tetrafluoromethane	FC(F)(F)F	dimethyl carbonate	0.96	1.59		1.28
carbon dioxide	O=C=O	dimethyl carbonate	-1.07	-0.59		-2.73
hydrogen sulfide	S	dimethyl carbonate	-1.55	-1.67		-2.69
methane	C	dimethyl carbonate	0.46	0.53	-0.30	-0.21
ethane	CC	dimethyl carbonate	-0.52	-0.37	-1.88	-1.63
ethene	C=C	dimethyl carbonate	-0.62	-0.72	-2.19	-2.34
cyclohexane	C1CCCCC1	dimethyl carbonate	-3.43	-3.84		-6.83
carbon tetrachloride	ClC(Cl)(Cl)Cl	dimethyl carbonate	-4.32	-4.52		-8.38
benzene	c1ccccc1	dimethyl carbonate	-3.96	-4.02		-7.37
helium	[He]	diethyl carbonate	2.05	2.32	3.28	2.68
neon	[Ne]	diethyl carbonate	1.88	2.21	2.59	2.37
argon	[Ar]	diethyl carbonate	0.78	1.18	0.49	0.66
krypton	[Kr]	diethyl carbonate	0.18	0.43	-0.63	-0.41
xenon	[Xe]	diethyl carbonate	-0.57	-0.23	-1.62	-1.29
nitrogen	N#N	diethyl carbonate	1.11	1.58		1.48
sulfur hexafluoride	F[S](F)(F)(F)(F)F	diethyl carbonate	-0.02	0.23	-0.57	-0.83
tetrafluoromethane	FC(F)(F)F	diethyl carbonate	0.91	1.56		1.24
hydrogen sulfide	S	diethyl carbonate	-1.44	-1.58		-2.51
ethane	CC	diethyl carbonate	-0.68	-0.44	-2.07	-2.00
hexane	CCCCCC	diethyl carbonate	-3.94	-3.46		-6.75
dodecane	CCCCCCCCCCCC	diethyl carbonate	-7.42	-7.54		-13.01
cyclohexane	C1CCCCC1	diethyl carbonate	-3.56	-3.90		-7.20
carbon tetrachloride	ClC(Cl)(Cl)Cl	diethyl carbonate	-4.28	-4.38		-8.30
benzene	c1ccccc1	diethyl carbonate	-4.41	-4.04	-8.08	-7.65

**Table S3.** Predicted and reference solvation free energies and solvation enthalpies in kcal/mol – testing set

Solute	Solute SMILES	Solvent	$\Delta^{\text{ref}}G_{\text{solv}}^{\circ}$	$\Delta^{\text{pred}}G_{\text{solv}}^{\circ}$	$\Delta^{\text{ref}}H_{\text{solv}}^{\circ}$	$\Delta^{\text{pred}}H_{\text{solv}}^{\circ}$
tetrafluoromethane	FC(F)(F)F	fluorobenzene	1.11	0.90		0.48
fluoromethane	CF	fluorobenzene	-0.90	-1.58		-3.49
difluoromethane	FCF	fluorobenzene	-1.01	-1.73		-3.41
argon	[Ar]	chlorobenzene	0.94	0.73	0.11	0.05
krypton	[Kr]	chlorobenzene	0.25	0.12	-0.73	-0.81
carbon monoxide	[C-]#[O+]	chlorobenzene	1.06	0.43	0.23	-0.46
ethane	CC	chlorobenzene	-0.80	-0.64	-2.36	-1.95
2,4-dimethylpentane	CC(C)CC(C)C	chlorobenzene	-4.24	-3.70		-6.75
1-pentene	CCCC=C	chlorobenzene	-3.01	-2.91		-5.39
fluoromethane	CF	chlorobenzene	-0.89	-1.27		-3.00
dichloromethane	ClCCl	chlorobenzene	-3.53	-3.59	-6.81	-6.58
tert-butyl bromide	CC(C)(C)Br	chlorobenzene	-3.93	-4.33		-7.91
methyl ethyl ketone	CCC(C)=O	chlorobenzene	-4.49	-4.80		-8.56
nitromethane	C[N+](=[O-])=O	chlorobenzene	-4.17	-5.14		-9.67
ethanol	CCO	chlorobenzene	-3.12	-3.65	-7.27	-7.58
1-butanol	CCCCO	chlorobenzene	-4.62	-5.06		-9.97
ethylbenzene	CCc1ccccc1	chlorobenzene	-5.84	-6.07	-10.28	-10.56
methyl ethyl ketone	CCC(C)=O	chlorobenzene	-4.53	-4.80		-8.56
pentyl acetate	CCCCCOC(C)=O	chlorobenzene	-6.55	-6.70		-11.75
methyl pentanoate	CCCCC(=O)OC	chlorobenzene	-5.83	-6.06		-10.58
ethylamine	CCN	chlorobenzene	-3.75	-3.33		-6.70
methanol	CO	chlorobenzene	-2.43	-3.04	-6.25	-6.49
1-heptanol	CCCCCCC	chlorobenzene	-6.75	-7.17		-13.40
2-butoxyethanol	CCCCOCCO	chlorobenzene	-6.17	-7.69		-14.69
helium	[He]	bromobenzene	2.61	1.95		1.87
argon	[Ar]	bromobenzene	1.09	0.89		0.12
krypton	[Kr]	bromobenzene	0.38	0.27		-0.93
radon	[Rn]	bromobenzene	-1.30	-0.81		-2.57
carbon dioxide	O=C=O	bromobenzene	-0.35	-0.69		-3.04
nitromethane	C[N+](=[O-])=O	bromobenzene	-4.15	-5.00		-9.83
2-chloroethanol	OCCCl	bromobenzene	-4.80	-5.82		-11.24
hydrogen sulfide	S	bromobenzene	-1.30	-1.91		-3.57
diethyl ether	CCOCC	bromobenzene	-3.83	-3.69		-7.21
methyl acetate	COC(C)=O	bromobenzene	-3.68	-4.26		-8.01
1-butanol	CCCCO	bromobenzene	-4.08	-4.83		-9.95
1-heptanol	CCCCCCC	bromobenzene	-6.66	-6.94		-13.39
butoxyethanol	CCCCOC(C)O	bromobenzene	-6.07	-6.09		-12.06
aniline	Nc1ccccc1	bromobenzene	-7.04	-7.19		-12.64
helium	[He]	iodobenzene	2.84	1.87		1.71
methane	C	iodobenzene	0.83	0.79		-0.60
propane	CCC	iodobenzene	-1.51	-0.78		-3.01
dimethyl ether	COC	iodobenzene	-2.03	-2.04		-5.04
butanone	CCC(C)=O	iodobenzene	-4.23	-4.19		-8.59
iodobenzene	Ic1ccccc1	iodobenzene	-7.12	-6.98		-12.48
methanol	CO	iodobenzene	-2.17	-2.37		-6.29
butan-1-ol	CCCCO	iodobenzene	-4.05	-4.35		-9.61
neon	[Ne]	hexafluorobenzene	1.55	1.54		1.17
tetrafluoromethane	FC(F)(F)F	hexafluorobenzene	0.02	1.45		1.57
perfluoropropane	FC(F)(F)C(F)(F)C(F)(F)F	hexafluorobenzene	-1.46	1.55		2.18
ethanol	CCO	hexafluorobenzene	-2.78	-2.27		-4.95

nitrogen	N#N	chloroform	1.19	0.89		0.58
pentane	CCCCC	chloroform	-3.22	-2.99	-5.79	-5.86
2,5-dimethylhexane	CC(C)CCC(C)C	chloroform	-4.86	-4.73		-8.60
chloromethane	CCl	chloroform	-2.48	-1.99		-4.25
1,1-dichloroethane	CC(Cl)Cl	chloroform	-4.11	-4.13		-7.39
1,1,2-trifluorotrichloroethane	FC(F)(Cl)C(F)(Cl)Cl	chloroform	-3.46	-3.28		-6.65
propanone	CC(C)=O	chloroform	-4.49	-4.01		-7.51
ethyl formate	CCOC=O	chloroform	-4.36	-4.22	-8.37	-7.80
methyl propanoate	CCC(=O)OC	chloroform	-5.48	-4.91	-10.77	-8.87
propylamine	CCCN	chloroform	-4.73	-3.99		-7.91
butylamine	CCCCN	chloroform	-5.27	-4.64		-9.05
triethylamine	CCN(CC)CC	chloroform	-5.76	-4.94	-11.09	-9.78
nitromethane	C[N+](=O)=O	chloroform	-4.62	-4.44	-9.01	-8.43
propanoic acid	CCC(O)=O	chloroform	-5.02	-5.36		-10.32
1-pentanol	CCCCCO	chloroform	-6.00	-5.51		-10.54
2-methyl-2-butanol	CCC(C)(C)O	chloroform	-5.10	-4.91		-9.84
2-methyl-1-pentanol	CCCC(C)CO	chloroform	-6.46	-5.98		-11.32
4-methyl-2-pentanol	CC(C)CC(C)O	chloroform	-5.88	-5.67		-10.91
3-ethyl-3-pentanol	CCC(O)(CC)CC	chloroform	-7.06	-6.01		-11.75
cyclohexanol	OC1CCCCC1	chloroform	-7.00	-6.79		-12.51
2-chloroethanol	OCCCl	chloroform	-5.73	-5.31		-9.79
2-ethoxyethanol	CCOCCO	chloroform	-6.26	-6.17		-11.97
dimethyl sulfoxide	C[S](C)=O	chloroform	-8.77	-7.99	-15.94	-14.45
thiourea	NC(N)=S	chloroform	-7.24	-7.95		-13.32
trimethyl phosphate	CO[P](=O)(OC)OC	chloroform	-9.51	-7.54		-11.10
tripropyl phosphate	CCCO[P](=O)(OCCC)OCCC	chloroform	-12.63	-10.19		-16.02
benzene	c1ccccc1	chloroform	-4.62	-4.57	-8.57	-8.28
1,2-dimethylbenzene	Cc1ccccc1C	chloroform	-6.23	-5.76		-10.12
phenylacetaldehyde	O=Cc1ccccc1	chloroform	-7.26	-7.69		-12.87
phenylacetone	N#CCc1ccccc1	chloroform	-8.12	-8.86		-14.09
aniline	Nc1ccccc1	chloroform	-7.71	-7.06	-13.41	-12.05
4-aminoacetophenone	CC(=O)c1ccc(N)cc1	chloroform	-11.10	-10.79		-18.46
2,4-dimethylaniline	Cc1ccc(N)c(C)c1	chloroform	-8.87	-8.04		-14.05
2-nitrotoluene	Cc1ccccc1[N+](=O)[O-]	chloroform	-8.21	-8.53		-14.56
2-methylphenol	Cc1ccccc1O	chloroform	-7.56	-7.20		-12.71
3-methylphenol	Cc1cccc(O)c1	chloroform	-7.49	-7.30		-12.81
3,5-dimethylphenol	Cc1cc(C)c(O)c1	chloroform	-8.46	-7.83		-13.61
2-ethylphenol	CCc1ccccc1O	chloroform	-8.39	-8.02		-14.15
2-isopropyl-5-methylphenol	CC(C)c1ccc(C)cc1O	chloroform	-9.63	-8.97		-15.62
2-fluorophenol	Oc1ccccc1F	chloroform	-6.07	-6.67		-12.76
4-chlorophenol	Oc1ccc(Cl)cc1	chloroform	-8.50	-7.71		-13.27
4-bromophenol	Oc1ccc(Br)cc1	chloroform	-8.59	-8.75		-15.39
4-iodophenol	Oc1ccc(I)cc1	chloroform	-9.74	-9.78		-16.61
3-nitrophenol	Oc1cccc(c1)[N+](=O)[O-]	chloroform	-10.31	-9.22		-16.20
2-phenylethanol	OCCc1ccccc1	chloroform	-8.58	-8.13		-14.25
pyridine	c1ccncc1	chloroform	-6.45	-5.95	-11.57	-10.05
2-ethylpyridine	CCc1ccncc1	chloroform	-7.42	-7.54		-12.84
n-methylpiperidine	CN1CCCCC1	chloroform	-5.74	-6.05		-11.26
argon	[Ar]	dichloromethane	0.96	0.54	0.92	-0.21
2-methylpentane	CCCC(C)C	dichloromethane	-3.53	-3.33	-5.48	-6.23
cyclohexane	C1CCCCC1	dichloromethane	-4.10	-4.18	-6.44	-7.42
ethyl acetate	CCOC(C)=O	dichloromethane	-5.23	-5.36	-8.99	-9.51
propanone	CC(C)=O	dichloromethane	-4.62	-4.31	-8.31	-7.83
acetonitrile	CC#N	dichloromethane	-4.70	-5.14	-8.57	-8.38
paracetamol	CC(=O)Nc1ccc(O)cc1	dichloromethane	-12.79	-12.64		-22.30
1,4-dioxane	C1COCCO1	dichloromethane	-5.83	-5.57	-10.46	-9.81
butanone	CCC(C)=O	dichloromethane	-5.27	-4.92	-9.08	-8.73
2-methyl-isopropanol	CC(C)(C)O	1-chlorobutane	-3.82	-4.50		-9.30
chloroform	ClC(Cl)Cl	1-chlorobutane	-4.07	-3.83		-6.88
dichloromethane	ClCCl	1-chlorobutane	-3.55	-3.27		-6.07
ethyl bromide	CCBr	1-chlorobutane	-3.50	-3.20		-6.26
chlorobenzene	Clc1ccccc1	1-chlorobutane	-5.59	-5.49		-9.41
dipropyl ether	CCOCCC	1-chlorobutane	-4.68	-5.07		-9.22
methyl butyl ether	CCCCOC	1-chlorobutane	-4.25	-4.49		-8.27
heptane	CCCCCCC	1-chlorobutane	-4.61	-4.04		-7.49
neon	[Ne]	carbon tetrachloride	1.87	1.77		1.51
nitrogen	N#N	carbon tetrachloride	1.08	0.91	0.56	0.61
pentane	CCCCC	carbon tetrachloride	-3.22	-3.11	-6.02	-6.07
hexane	CCCCCC	carbon tetrachloride	-4.07	-3.83	-7.11	-7.21
heptane	CCCCCCC	carbon tetrachloride	-4.75	-4.55	-8.24	-8.35
octane	CCCCCCCC	carbon tetrachloride	-5.52	-5.28	-9.35	-9.56
2,3,4-trimethylpentane	CC(C)(C)C(C)C	carbon tetrachloride	-5.07	-4.81		-8.74
nonane	CCCCCCCCC	carbon tetrachloride	-6.20	-5.97	-10.32	-10.60
cycloheptane	C1CCCCC1	carbon tetrachloride	-5.30	-4.97	-9.06	-8.83
cyclooctane	C1CCCCCCC1	carbon tetrachloride	-6.10	-5.64	-10.27	-9.90
ethylcyclohexane	CCC1CCCCC1	carbon tetrachloride	-5.57	-5.56		-9.76
cis-decalin	C1CC[C@@H]2CCCC[C@H]2C1	carbon tetrachloride	-7.23	-7.16	-12.14	-11.97
isobutene	CC(C)=C	carbon tetrachloride	-2.44	-2.25		-4.70
1,2-dichloropropane	CC(Cl)CCl	carbon tetrachloride	-4.65	-4.73		-8.44
tetrachloroethene	ClC(Cl)=C(Cl)Cl	carbon tetrachloride	-5.48	-4.81		-8.70
bromoethane	CCBr	carbon tetrachloride	-3.45	-3.31		-6.60
iodoethane	CCl	carbon tetrachloride	-4.17	-4.07		-7.22
1-methoxy-2-ethoxyethane	CCOCCOC	carbon tetrachloride	-5.85	-4.81		-8.76

2-octanone	CCCCCCC(C)=O	carbon tetrachloride	-6.70	-6.79	-12.11	-11.94
methylamine	CN	carbon tetrachloride	-2.33	-1.99		-4.28
methanol	CO	carbon tetrachloride	-2.05	-1.79	-4.73	-4.18
carbon disulfide	S=C=S	carbon tetrachloride	-3.63	-3.92		-5.26
tetramethylstannane	C[Sn](C)(C)C	carbon tetrachloride	-4.42	-4.26	-7.57	-7.50
benzene	c1ccccc1	carbon tetrachloride	-4.42	-4.25	-7.96	-7.90
chlorobenzene	Clc1ccccc1	carbon tetrachloride	-5.65	-5.35	-9.64	-9.50
isobutanol	CC(C)CO	carbon tetrachloride	-3.94	-4.06		-7.96
2-butanol	CCC(C)O	carbon tetrachloride	-3.89	-3.98		-7.86
3-methyl-3-hexanol	CCCC(C)(O)CC	carbon tetrachloride	-5.98	-5.69		-10.83
3-methyl-2-hexanol	CCCC(C)C(C)O	carbon tetrachloride	-5.93	-5.71		-10.69
cyclohexene	C1CCC=CC1	carbon tetrachloride	-4.58	-4.19		-7.59
germanium tetrachloride	Cl[Ge](Cl)(Cl)Cl	carbon tetrachloride	-4.27	-3.00		-6.02
iodobenzene	Ic1ccccc1	carbon tetrachloride	-7.03	-6.68	-11.47	-11.12
2,3-dimethylbuta-1,3-diene	CC(=C)C(C)=C	carbon tetrachloride	-4.41	-3.67		-6.94
isobutene	CC(C)=C	carbon tetrachloride	-2.71	-2.25		-4.70
propyl acetate	CCCOC(C)=O	carbon tetrachloride	-4.97	-4.94		-9.14
propylamine	CCCN	carbon tetrachloride	-3.59	-3.31		-6.63
butylamine	CCCCN	carbon tetrachloride	-4.29	-4.02	-8.49	-7.83
2-methylphenol	Cc1ccccc1O	carbon tetrachloride	-6.79	-6.14		-10.93
1,3-dimethylbenzene	Cc1ccccc1C	carbon tetrachloride	-5.70	-5.57		-9.91
methoxybenzene	COc1ccccc1	carbon tetrachloride	-5.78	-5.78		-10.21
2-chloroaniline	Nc1ccccc1Cl	carbon tetrachloride	-7.27	-7.38		-12.40
2-methoxyaniline	COc1ccccc1N	carbon tetrachloride	-7.79	-8.71		-15.79
cyclopentanone	O=C1CCCC1	carbon tetrachloride	-5.28	-4.99	-9.89	-8.90
allyl alcohol	OCC=C	carbon tetrachloride	-3.55	-3.34		-6.67
3-aminophenol	Nc1ccccc1O	carbon tetrachloride	-8.55	-8.05		-14.50
octane	CCCCCCCC	bromoethane	-5.32	-4.81		-8.78
nitromethane	C[N+](=[O-])=O	bromoethane	-4.44	-4.69		-8.73
ethane	CC	methylene iodide	0.34	-0.07		-3.04
hexane	CCCCCC	methylene iodide	-2.06	-3.21		-8.02
heptane	CCCCCCC	methylene iodide	-2.85	-3.94		-9.21
1,4-dioxane	C1COCCO1	methylene iodide	-4.94	-4.69		-10.25
methyl ethyl ketone	CCC(C)=O	methylene iodide	-3.83	-4.48		-10.24
methyl acetate	COC(C)=O	methylene iodide	-3.16	-3.55		-8.39
1-butanol	CCCCO	methylene iodide	-4.13	-4.28		-10.35
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	methylene iodide	-5.40	-6.17		-12.64
4-chlorotoluene	Cc1ccc(Cl)cc1	methylene iodide	-5.46	-6.27		-12.72
octane	CCCCCCCC	dibromomethane	-4.67	-4.77		-9.62
dichloromethane	ClCCl	dibromomethane	-3.85	-3.12		-6.70
oxygen	O=O	diethyl ether	0.48	0.48		-0.41
nitrogen	N#N	diethyl ether	0.75	0.81		0.52
2-methylpropane	CC(C)C	diethyl ether	-2.33	-2.54		-5.27
1,2-dichloroethane	ClCCCl	diethyl ether	-4.45	-4.66		-8.63
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	diethyl ether	-4.13	-5.42		-9.76
propanone	CC(C)=O	diethyl ether	-3.51	-3.71		-7.10
triethylamine	CCN(CC)CC	diethyl ether	-4.45	-4.56	-8.10	-8.15
oxygen	O=O	dibutyl ether	0.78	0.68		-0.06
cyclohexane	C1CCCCC1	dibutyl ether	-4.11	-4.10	-7.74	-7.61
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	dibutyl ether	-4.08	-5.05		-9.37
tetrahydrofuran	C1CCOC1	dibutyl ether	-3.81	-3.92	-7.42	-7.45
tetramethylstannane	C[Sn](C)(C)C	dibutyl ether	-4.26	-4.07		-7.26
toluene	Cc1ccccc1	dibutyl ether	-4.88	-4.92	-9.05	-9.07
octane	CCCCCCCC	diisopropyl ether	-5.24	-5.45		-9.98
1-hexene	CCCCC=C	diisopropyl ether	-3.86	-4.54		-8.79
ethanol	CCO	diisopropyl ether	-3.65	-4.11		-9.05
nitromethane	C[N+](=[O-])=O	diisopropyl ether	-3.83	-3.41		-7.10
2,2,4-trimethylpentane	CC(C)CC(C)C	methyl <i>tert</i> -butyl ether	-4.65	-4.55		-8.39
CF <sub>3</sub> CHBrCl	C(F)(F)(F)C(Br)(Cl)	methyl <i>tert</i> -butyl ether	-4.69	-4.41		-8.68
1,2-difluorotetrachloroethane	FC(Cl)(Cl)C(F)(Cl)Cl	methyl <i>tert</i> -butyl ether	-4.68	-5.45		-10.03
diethyl carbonate	CCOC(=O)OCC	methyl <i>tert</i> -butyl ether	-5.35	-5.70		-10.15
propan-1-ol	CCCO	methyl <i>tert</i> -butyl ether	-4.60	-5.06		-10.50
oxygen	O=O	dipropyl ether	0.65	0.61		-0.10
butan-1-ol	CCCCO	dipropyl ether	-4.94	-5.11		-10.54
butan-2-ol	CCC(C)O	dipropyl ether	-4.40	-4.98		-10.37
hexan-1-ol	CCCCCCO	dipropyl ether	-6.31	-6.31		-12.33
dichloromethane	ClCCl	dipropyl ether	-3.51	-3.42		-6.88
neon	[Ne]	tetrahydrofuran	2.03	1.96	1.68	1.90
argon	[Ar]	tetrahydrofuran	0.76	0.69	-0.01	0.05
deuterium	[H][H]	tetrahydrofuran	1.47	1.33	1.44	0.88
pentane	CCCCC	tetrahydrofuran	-3.18	-3.07		-5.83
2,4-dimethylpentane	CC(C)CC(C)C	tetrahydrofuran	-4.13	-4.12		-7.48
octane	CCCCCCCC	tetrahydrofuran	-5.25	-5.04	-8.97	-8.85
2,2,4-trimethylpentane	CC(C)CC(C)C	tetrahydrofuran	-4.65	-4.17	-7.86	-7.46
methylcyclohexane	CC1CCCCC1	tetrahydrofuran	-4.67	-4.45	-7.86	-7.50
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	tetrahydrofuran	-4.35	-5.86		-10.36
butanone	CCC(C)=O	tetrahydrofuran	-4.54	-4.57		-8.16
ethanol	CCO	tetrahydrofuran	-4.56	-4.57	-9.08	-9.60
propan-2-ol	CC(C)O	tetrahydrofuran	-4.69	-5.00		-10.21
toluene	Cc1ccccc1	tetrahydrofuran	-5.44	-5.42	-9.27	-9.51
<i>tert</i> -butylbenzene	CC(C)(C)c1ccccc1	tetrahydrofuran	-6.94	-7.05		-12.12
chlorobenzene	Clc1ccccc1	tetrahydrofuran	-6.04	-5.95	-10.46	-10.26
bromobenzene	Br1ccccc1	tetrahydrofuran	-6.45	-6.11		-10.43

iodobenzene	Ic1ccccc1	tetrahydrofuran	-7.38	-6.91		-11.14
nitromethane	C[N+](=O)[O-]	bis(2-ethoxyethyl) ether	-4.84	-4.33		-9.59
helium	[He]	tetrahydrofuran	2.27	2.12		2.23
sulfur hexafluoride	F[S](F)(F)(F)(F)F	tetrahydrofuran	0.05	0.27		-1.08
2-methylpropene	CC(C)=C	tetrahydrofuran	-2.48	-2.51		-5.05
1,3-butadiene	C=CC=C	tetrahydrofuran	-2.69	-2.92		-5.71
neon	[Ne]	anisole	2.31	2.00		1.97
tetrafluoromethane	FC(F)(F)F	anisole	1.52	1.17		0.34
sulfur hexafluoride	F[S](F)(F)(F)(F)F	anisole	0.62	0.52		-0.98
pentane	CCCCC	anisole	2.00	-2.54		-4.88
nonane	CCCCCCCCC	anisole	-5.34	-5.55		-9.78
2-methyl-1,3-butadiene	CC(=C)C=C	anisole	-3.14	-3.04		-5.71
tetrachloromethane	ClC(Cl)(Cl)Cl	anisole	-4.17	-4.73		-8.72
bromoethane	CCBr	anisole	-3.44	-3.26		-6.30
3-methyl-1-butanol	CC(C)CCO	anisole	-5.14	-5.89		-11.63
anisole	COc1ccccc1	anisole	-6.38	-6.35		-11.11
n-butane	CCCC	N-methyl-2-pyrrolidone	-1.56	-1.30		-3.69
2,2-dimethylbutane	CCC(C)(C)C	N-methyl-2-pyrrolidone	-2.13	-2.03	-4.57	-4.94
2,2,3-trimethylbutane	CC(C)(C)(C)C	N-methyl-2-pyrrolidone	-2.78	-2.43	-5.97	-5.67
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	N-methyl-2-pyrrolidone	-3.12	-2.90	-5.94	-6.45
nonane	CCCCCCCCC	N-methyl-2-pyrrolidone	-4.28	-4.19		-8.28
methylcyclohexane	CC1CCCCC1	N-methyl-2-pyrrolidone	-3.59	-3.41	-7.23	-6.83
propene	CC=C	N-methyl-2-pyrrolidone	-1.24	-1.14		-3.42
2-methylbuta-1,3-diene	CC(=C)C=C	N-methyl-2-pyrrolidone	-2.86	-2.74		-5.94
trans-penta-1,3-diene	C/C=C/C=C	N-methyl-2-pyrrolidone	-3.04	-2.79		-5.90
cyclohexene	C1CCC=CC1	N-methyl-2-pyrrolidone	-3.70	-3.49		-6.94
octyne	CCCCCCC#C	N-methyl-2-pyrrolidone	-4.87	-4.51		-8.65
trifluoromethane	FC(F)F	N-methyl-2-pyrrolidone	-1.35	-0.32		-1.84
1-chloro-1,1-difluoroethane	CC(F)(F)Cl	N-methyl-2-pyrrolidone	-2.13	-2.81		-5.69
1-chloro-2,2-difluoroethane	FC(F)=CCl	N-methyl-2-pyrrolidone	-2.26	-1.72		-4.57
butanal	CCCC=O	N-methyl-2-pyrrolidone	-4.16	-4.00		-7.70
methyl acetate	COC(C)=O	N-methyl-2-pyrrolidone	-3.71	-4.02	-7.31	-7.72
methanol	CO	N-methyl-2-pyrrolidone	-4.68	-3.65	-9.48	-9.02
tert-butanol	CC(C)(C)O	N-methyl-2-pyrrolidone	-5.12	-4.47		-10.53
N-methyl-2-pyrrolidone	CN1CCCC1=O	N-methyl-2-pyrrolidone	-7.67	-7.64	-13.12	-14.62
sulfur hexafluoride	F[S](F)(F)(F)(F)F	methylformamide	1.02	-0.70		-2.92
nonane	CCCCCCCCC	methylformamide	-3.82	-3.52	-9.42	-6.68
ethene	C=C	methylformamide	-0.20	-1.27		-3.45
cis-penta-1,3-diene	C/C=C/C=C	methylformamide	-2.67	-2.91		-5.91
trans-penta-1,3-diene	C/C=C/C=C	methylformamide	-2.59	-2.96		-6.03
ethanol	CCO	methylformamide	-4.86	-4.44	-9.26	-10.21
benzene	c1ccccc1	methylformamide	-3.83	-3.93	-7.82	-7.51
helium	[He]	n-methylacetamide	2.46	1.74		1.14
n-pentane	CCCCC	n-methylacetamide	-2.17	-2.01		-4.60
trans-penta-1,3-diene	C/C=C/C=C	n-methylacetamide	-2.99	-2.85		-5.96
1,2-dichloroethane	ClCCCl	n-methylacetamide	-4.45	-4.43		-8.74
ethyl t-butyl ether	CCOC(C)(C)C	n-methylacetamide	-3.40	-3.51		-7.05
tetrahydrofuran	C1CCOC1	n-methylacetamide	-3.87	-4.08		-8.00
acetaldehyde	CC=O	n-methylacetamide	-2.85	-3.31		-6.96
2-methylpropanal	CC(C)C=O	n-methylacetamide	-3.68	-3.96		-7.78
propanone	CC(C)=O	n-methylacetamide	-3.67	-3.90		-7.90
methyl formate	COC=O	n-methylacetamide	-3.15	-4.35		-8.49
methyl acetate	COC(C)=O	n-methylacetamide	-3.62	-4.74		-8.94
propyl acetate	CCCOC(C)=O	n-methylacetamide	-4.54	-5.18		-9.53
ethanol	CCO	n-methylacetamide	-4.98	-4.31		-10.10
ethylbenzene	CCc1ccccc1	n-methylacetamide	-5.05	-4.70		-8.66
chlorobenzene	Clc1ccccc1	n-methylacetamide	-5.17	-5.18		-9.67
propane	CCC	formamide	0.19	-0.44		-3.35
n-butane	CCCC	formamide	-0.12	-0.80		-3.78
n-hexane	CCCCCC	formamide	-0.53	-1.62		-4.92
n-heptane	CCCCCCC	formamide	-0.90	-2.22		-5.88
cyclohexane	C1CCCCC1	formamide	-1.35	-2.73	-6.17	-6.66
hexanal	CCCCCCC=O	formamide	-4.02	-4.36		-9.11
nonan-2-one	CCCCCCCC(C)=O	formamide	-5.43	-5.75		-11.27
methyl isopentyl ketone	CC(C)CCCC(C)=O	formamide	-4.52	-4.65		-9.66
methyl isohexyl ketone	CC(C)CCCC(C)=O	formamide	-4.76	-5.04		-10.28
methyl formate	COC=O	formamide	-3.08	-3.41		-7.69
heptyl acetate	CCCCCCCOC(C)=O	formamide	-4.84	-5.52		-11.18
pentan-1-ol	CCCCCO	formamide	-5.65	-5.19	-12.53	-12.68
heptan-1-ol	CCCCCCCO	formamide	-6.38	-6.08	-14.38	-14.04
benzene	c1ccccc1	formamide	-2.69	-3.15	-7.03	-7.21
ethylbenzene	CCc1ccccc1	formamide	-3.26	-4.25	-8.80	-8.81
hydrogen	[H][H]	ethylbenzene	1.62	1.58		1.27
hexane	CCCCCC	ethylbenzene	-3.80	-3.61		-6.56
octane	CCCCCCCC	ethylbenzene	-4.97	-5.11		-9.03
methylcyclohexane	CC1CCCCC1	ethylbenzene	-4.56	-4.75		-8.21
2-hexanone	CCCCC(C)=O	ethylbenzene	-5.48	-5.40		-9.49
propan-1-ol	CCCO	ethylbenzene	-3.68	-3.47		-6.92
butan-1-ol	CCCCO	ethylbenzene	-4.43	-4.16		-8.04
1-pentanol	CCCCCO	ethylbenzene	-5.18	-4.88		-9.22
2-methylpropan-1-ol	CC(C)CO	ethylbenzene	-3.77	-4.00		-7.78
propionitrile	CCC#N	ethylbenzene	-4.17	-4.01		-6.54
propylamine	CCCN	ethylbenzene	-3.44	-3.24		-6.36



5-methylfurfural	Cc1oc(C=O)cc1	ethylbenzene	-6.74	-6.50		-11.43
sulfur hexafluoride	F[S](F)(F)(F)(F)F	<i>m</i> -xylene	0.19	0.47		-0.73
2-methylpropane	CC(C)C	<i>m</i> -xylene	-2.07	-1.99		-4.02
ethene	C=C	<i>m</i> -xylene	-0.61	-0.72		-2.02
1-propene	CC=C	<i>m</i> -xylene	-1.58	-1.49		-3.26
<i>trans</i> -2-butene	C/C=C/C	<i>m</i> -xylene	-2.50	-2.26		-4.47
1-hexene	CCCCC=C	<i>m</i> -xylene	-3.74	-3.63		-6.61
fluoromethane	CF	<i>m</i> -xylene	-0.74	-0.50		-1.69
dimethyl ether	COC	<i>m</i> -xylene	-2.05	-2.17		-4.38
propan-1-ol	CCCO	<i>m</i> -xylene	-3.72	-3.42		-6.88
butan-2-ol	CCC(C)O	<i>m</i> -xylene	-4.14	-4.01		-7.86
pentan-1-ol	CCCCCO	<i>m</i> -xylene	-5.21	-4.93		-9.37
<i>trans</i> -2-butene	C/C=C\C	<i>m</i> -xylene	-2.47	-2.24		-4.45
1,1-difluoroethane	CC(F)F	<i>o</i> -xylene	-1.62	-1.64		-3.40
dimethyl ether	COC	<i>o</i> -xylene	-2.04	-2.19		-4.42
butan-2-ol	CCC(C)O	<i>o</i> -xylene	-4.19	-4.09		-8.08
3-methyl-1-butanol	CC(C)CCO	<i>o</i> -xylene	-4.94	-4.90		-9.32
pentan-1-ol	CCCCCO	<i>o</i> -xylene	-5.21	-5.02		-9.60
2-chloroethanol	OCCCl	<i>o</i> -xylene	-4.74	-4.74		-8.83
<i>o</i> -xylene	Cc1ccccc1C	<i>o</i> -xylene	-5.95	-5.72		-10.11
oxygen	O=O	<i>p</i> -xylene	0.83	0.87		0.28
sulfur hexafluoride	F[S](F)(F)(F)(F)F	<i>p</i> -xylene	0.19	0.45		-0.72
<i>trans</i> -2-butene	C/C=C\C	<i>p</i> -xylene	-2.48	-2.25		-4.46
2-methylprop-1-ene	CC(C)=C	<i>p</i> -xylene	-2.32	-2.12		-4.24
acetylene	C#C	<i>p</i> -xylene	-0.80	-0.82		-2.24
iodomethane	CI	<i>p</i> -xylene	-3.47	-3.41		-5.98
1,1-difluoroethane	CC(F)F	<i>p</i> -xylene	-1.62	-1.50		-3.16
acetonitrile	CC#N	<i>p</i> -xylene	-3.44	-3.15		-5.21
butan-2-ol	CCC(C)O	<i>p</i> -xylene	-4.23	-3.94		-7.72
2-methylpropan-2-ol	CC(C)(C)O	<i>p</i> -xylene	-3.36	-3.75		-7.61
benzene	c1ccccc1	<i>p</i> -xylene	-4.37	-4.18		-7.60
chlorine	ClCl	<i>p</i> -xylene	-2.09	-1.32		-3.01
helium	[He]	toluene	2.25	1.97	2.42	1.98
neon	[Ne]	toluene	2.04	1.86	1.97	1.69
krypton	[Kr]	toluene	0.15	-0.01	-0.89	-0.82
carbon monoxide	[C-]#[O+]	toluene	1.01	0.64	0.45	0.04
carbon dioxide	O=C=O	toluene	-0.50	-0.56	-2.52	-2.07
chlorine	ClCl	toluene	-2.28	-1.53	-5.73	-3.23
methane	C	toluene	0.35	0.03	-1.21	-0.78
2-methylpentane	CCCC(C)C	toluene	-3.62	-3.59		-6.41
<i>trans</i> -2-butene	C/C=C\C	toluene	-2.55	-2.38		-4.51
trifluoromethane	FC(F)F	toluene	-0.29	-0.32		-1.39
trichloromethane	ClC(Cl)Cl	toluene	-4.26	-4.08		-7.16
iodoethane	CCI	toluene	-4.21	-4.20		-7.05
dimethyl ether	COC	toluene	-2.16	-2.35		-4.57
di-isopropylether	CC(C)OC(C)C	toluene	-3.98	-4.67		-8.30
furan	c1ccccc1	toluene	-3.34	-3.88		-7.02
pentan-2-one	CCCC(C)=O	toluene	-5.02	-4.88		-8.64
heptan-2-one	CCCCCC(C)=O	toluene	-6.30	-6.14		-10.59
acetonitrile	CC#N	toluene	-3.65	-3.61	-7.46	-6.03
dimethylamine	CNC	toluene	-2.68	-2.63		-5.26
nitroethane	CC[N+](=O)=O	toluene	-4.62	-4.66		-8.86
water	O	toluene	-1.69	-1.85	-4.25	-4.59
butan-1-ol	CCCCO	toluene	-4.54	-4.22		-7.99
3-methylbutan-1-ol	CC(C)CCO	toluene	-5.00	-4.88		-9.05
2-chloroethanol	OCCCl	toluene	-4.67	-4.64		-8.48
4-methylaniline	Cc1ccc(N)cc1	toluene	-7.39	-7.09		-12.04
neon	[Ne]	benzene	2.09	1.84	2.50	1.69
argon	[Ar]	benzene	0.85	0.48	0.30	-0.13
nitric oxide	[N]=O	benzene	0.71	0.19	0.59	-0.38
2,5-dimethylhexane	CC(C)CCC(C)C	benzene	-4.77	-4.98		-8.40
2,3,4-trimethylpentane	CC(C)C(C)(C)C	benzene	-4.82	-4.84		-8.21
ethyne	C#C	benzene	-0.98	-1.11		-2.35
fluoromethane	CF	benzene	-0.75	-0.95		-2.24
chloroethane	CCCl	benzene	-3.04	-2.83	-6.12	-5.17
toluene	Cc1ccccc1	benzene	-5.32	-5.32	-9.00	-9.18
methyl ethyl ketone	CCC(C)=O	benzene	-4.46	-4.41	-8.19	-7.95
2-pentanone	CCCC(C)=O	benzene	-5.13	-5.08	-8.99	-8.99
cyclohexanone	O=C1CCCCC1	benzene	-6.41	-6.20	-11.03	-10.68
water	O	benzene	-1.96	-1.94	-4.68	-4.56
radon	[Rn]	ethyl acetate	-1.10	-1.02		-2.36
oxygen	O=O	ethyl acetate	0.90	0.01		-1.89
carbon monoxide	[C-]#[O+]	ethyl acetate	0.82	0.41		-0.51
pentane	CCCCC	ethyl acetate	-2.85	-2.81	-5.09	-5.42
2,5-dimethylhexane	CC(C)CCC(C)C	ethyl acetate	-4.31	-4.40		-7.76
cyclohexane	C1CCCCC1	ethyl acetate	-3.77	-3.86	-6.54	-6.73
propene	CC=C	ethyl acetate	-1.51	-1.71		-3.83
trichloromethane	ClC(Cl)Cl	ethyl acetate	-4.61	-4.10		-7.52
bromoethane	CCBr	ethyl acetate	-3.53	-3.22		-6.39
propionitrile	CCC#N	ethyl acetate	-4.68	-4.43		-7.03
triethylamine	CCN(CC)CC	ethyl acetate	-4.27	-4.14	-7.60	-7.47
nitromethane	C[N+](=O)=O	ethyl acetate	-4.92	-4.48		-9.13
ethanol	CCO	ethyl acetate	-4.12	-4.14	-8.46	-9.04

oxygen	O=O	methyl acetate	0.77	0.08	0.34	-1.71
sulfur dioxide	O=[S]=O	methyl acetate	-3.08	-3.58		-8.18
methane	C	methyl acetate	0.31	0.41	-0.33	-0.25
octane	CCCCCCCC	methyl acetate	-4.49	-4.58	-7.39	-7.87
cyclohexane	C1CCCCC1	methyl acetate	-3.60	-3.78		-6.45
chloroform	ClC(Cl)Cl	methyl acetate	-4.67	-4.24		-7.69
1,1,2-trichlorotrifluoroethane	FC(F)(Cl)C(F)(Cl)Cl	methyl acetate	-3.38	-3.96		-7.89
2-bromo-2-chloro-1,1,1-trifluoroethane	FC(F)(F)C(Cl)Br	methyl acetate	-4.61	-3.65		-6.81
methanol	CO	methyl acetate	-3.77	-3.62		-8.11
2-methoxyethanol	COCCO	methyl acetate	-5.46	-5.41		-10.95
nitrogen	N#N	butyl acetate	1.09	1.20		0.83
pentane	CCCCC	butyl acetate	-2.94	-2.71		-5.48
2,4-dimethylpentane	CC(C)CC(C)C	butyl acetate	-3.81	-3.75		-7.02
2,5-dimethylhexane	CC(C)CCC(C)C	butyl acetate	-4.46	-4.48		-8.16
2,3,4-trimethylpentane	CC(C)(C)C(C)C	butyl acetate	-4.56	-4.15		-7.56
cyclohexane	C1CCCCC1	butyl acetate	-3.91	-3.94		-7.15
1-heptene	CCCCC=C	butyl acetate	-4.28	-4.53		-8.48
2-butanol	CCC(C)O	butyl acetate	-4.90	-4.67		-9.75
octane	CCCCCCCC	propyl acetate	-4.85	-4.63		-8.23
nonane	CCCCCCCCC	propyl acetate	-5.47	-5.44		-9.55
1-chlorobutane	CCCCCl	propyl acetate	-4.31	-4.13		-7.89
toluene	Cc1ccccc1	propyl acetate	-5.10	-4.98		-8.89
m-xylene	Cc1cccc(C)c1	propyl acetate	-5.72	-5.47		-9.60
propyl acetate	CCCOC(C)=O	propyl acetate	-5.02	-5.16		-9.57
carbon monoxide	[C-]#[O+]	pentyl acetate	0.91	0.57		-0.53
1-hexene	CCCCC=C	pentyl acetate	-3.75	-3.81		-7.44
1,7-octadiene	C=CCCCC=C	pentyl acetate	-5.03	-5.49		-10.14
toluene	Cc1ccccc1	pentyl acetate	-5.06	-4.90		-9.00
p-xylene	Cc1ccc(C)cc1	pentyl acetate	-5.71	-5.55		-10.02
1,4-dioxane	C1COCCO1	pentyl acetate	-4.85	-4.67		-8.56
1-propanol	CCCO	pentyl acetate	-4.62	-4.39		-9.60
hexyl acetate	CCCCCOC(C)=O	hexyl acetate	-6.79	-6.87		-12.52
carbon dioxide	O=C=O	2-methoxyethanol	-0.65	-0.37		-2.68
hexane	CCCCC	2-methoxyethanol	-2.71	-2.76	-5.88	-5.69
2-chloro-2-methylpropane	CC(C)(C)Cl	2-methoxyethanol	-3.31	-3.36	-6.41	-6.70
butanone	CCC(C)=O	2-methoxyethanol	-4.32	-3.62		-6.69
o-xylene	Cc1ccccc1C	2-methoxyethanol	-5.26	-5.20	-9.78	-9.43
propan-2-ol	CC(C)O	2-methoxyethanol	-4.66	-4.19		-9.38
isopropanol	CC(C)O	2-ethoxyethanol	-4.87	-3.99		-9.07
methyl formate	COC=O	2-ethoxyethanol	-3.08	-2.64		-5.51
methyl acetate	COC(C)=O	2-ethoxyethanol	-3.69	-3.09		-6.10
benzene	c1ccccc1	2-ethoxyethanol	-4.13	-3.85		-7.33
hydrogen	[H][H]	2-butoxyethanol	1.67	1.24		0.28
carbon dioxide	O=C=O	2-butoxyethanol	-0.26	0.23		-1.66
undecane	CCCCCCCCCCC	2-butoxyethanol	-6.17	-6.50		-11.82
benzene	c1ccccc1	2-butoxyethanol	3.00	-3.80		-7.31
fluorobenzene	Fc1ccccc1	2-butoxyethanol	-4.30	-4.12		-8.02
chlorobenzene	Clc1ccccc1	2-butoxyethanol	-5.33	-5.42		-10.01
carbon dioxide	O=C=O	diethylene glycol	-0.28	0.19		-2.96
octane	CCCCCCCC	diethylene glycol	-2.38	-3.26		-7.73
nonane	CCCCCCCCC	diethylene glycol	-2.80	-4.12		-9.15
decane	CCCCCCCCC	diethylene glycol	-3.21	-4.86		-10.34
undecane	CCCCCCCCCCC	diethylene glycol	-3.68	-5.43		-11.31
dodecane	CCCCCCCCCCCC	diethylene glycol	-4.01	-6.09		-12.36
cyclohexane	C1CCCCC1	diethylene glycol	-2.18	-2.49		-6.06
1-hexene	CCCCC=C	diethylene glycol	-1.66	-2.78		-7.07
1,7-octadiene	C=CCCCC=C	diethylene glycol	-2.91	-4.15		-9.02
1,2-dichloropropane	CC(Cl)CCl	diethylene glycol	-3.97	-4.62		-9.69
o-xylene	Cc1ccccc1C	diethylene glycol	-4.52	-4.63		-9.78
p-xylene	Cc1ccc(C)cc1	diethylene glycol	-4.26	-4.68		-9.84
butyl acetate	CCCCOC(C)=O	diethylene glycol	-4.32	-4.54		-9.75
ethanol	CCO	diethylene glycol	-4.67	-3.17		-8.97
1-hexyne	CCCCC#C	diethylene glycol	-2.80	-3.03		-7.28
methanol	CO	diethylene glycol	-4.39	-2.75		-8.27
1-propanol	CCCO	diethylene glycol	-4.94	-3.73		-9.89
propane	CCC	triethylene glycol	-2.01	0.06		-1.41
heptane	CCCCCCC	triethylene glycol	-4.69	-2.45		-5.45
decane	CCCCCCCCC	triethylene glycol	-6.47	-4.59		-8.90
methylcyclohexane	CC1CCCCC1	triethylene glycol	-4.18	-2.79		-5.59
2,4,4-trimethyl-1-pentene	CC(=C)CC(C)(C)C	triethylene glycol	-4.35	-2.42		-5.34
cyclohexene	C1CCC=CC1	triethylene glycol	-3.10	-2.48		-5.08
1-heptyne	CCCCC#C	triethylene glycol	-3.84	-3.43		-7.12
1,2-dichloropropane	CC(Cl)CCl	triethylene glycol	-2.72	-4.44		-8.76
isopropylbromide	CC(C)Br	triethylene glycol	-2.29	-2.69		-6.16
m-xylene	Cc1cccc(C)c1	triethylene glycol	-3.62	-4.05		-7.70
nitromethane	[N+](=[O-])=O	triethylene glycol	-0.83	-4.12		-9.18
krypton	[Kr]	pentane	-0.30	-0.29		-1.18
propane	CCC	pentane	-1.81	-1.78		-3.77
2-methylpentane	CCCC(C)C	pentane	-3.94	-3.83		-6.92
propene	CC=C	pentane	-1.79	-1.75		-3.65
dichloromethane	ClCCl	pentane	-2.91	-2.82		-5.23
methyl acetate	COC(C)=O	pentane	-2.94	-3.42		-6.62

radon	[Rn]	hexane	-1.55	-1.24	-3.03	-2.79
hydrogen	[H][H]	hexane	1.24	1.34	1.22	0.89
carbon monoxide	[C-]#[O+]	hexane	0.66	0.46		-0.34
iodine	I	hexane	-4.67	-5.38		-8.68
heptane	CCCCCCC	hexane	-4.77	-4.60	-8.74	-8.29
2,3,4-trimethylpentane	CC(C)(C)C(C)C	hexane	-5.02	-4.94		-8.82
undecane	CCCCCCCCCCC	hexane	-7.56	-7.44	-13.44	-12.79
cyclohexane	C1CCCCC1	hexane	-4.23	-4.11	-7.75	-7.29
isobutene	CC(C)=C	hexane	-0.64	-2.39		-4.88
propene	CC=C	hexane	-1.75	-1.76		-3.92
isobutene	CC(C)=C	hexane	-2.43	-2.39		-4.88
tetrafluoromethane	FC(F)(F)F	hexane	0.50	0.40	-0.35	-0.75
chloroethane	CCCl	hexane	-2.60	-2.40		-4.81
1,2-dichloroethane	ClCCCl	hexane	-3.75	-3.68	-6.99	-6.66
furan	c1ccoc1	hexane	-2.90	-3.54	-5.70	-6.71
3,3-dimethylbutan-2-one	CC(=O)C(C)(C)C	hexane	-4.34	-4.36		-7.88
cyclohexanone	O=C1CCCCC1	hexane	-4.98	-5.34		-9.38
methyl acetate	COC(C)=O	hexane	-2.93	-3.22	-5.11	-6.27
butyronitrile	CCCC#N	hexane	-3.75	-4.13	-7.57	-7.03
dimethylamine	CNC	hexane	-2.48	-2.68		-5.64
trimethylamine	CN(C)C	hexane	-2.63	-3.14		-6.37
decan-1-ol	CCCCCCCCCO	hexane	-7.69	-8.02		-14.02
2-ethoxyethanol	CCOCCO	hexane	-4.01	-4.60		-8.84
tetraethylsilicon	CC[Si](CC)(CC)CC	hexane	-6.33	-5.30		-9.11
chlorobenzene	Clc1ccccc1	hexane	-5.21	-5.17	-9.09	-9.10
fluorobenzene	Fc1ccccc1	hexane	-4.15	-4.26		-7.92
4-methylaniline	Cc1ccc(N)cc1	hexane	-6.06	-6.34		-10.91
hydrogen	[H][H]	heptane	1.29	1.41	0.90	0.95
deuterium	[H][H]	heptane	1.27	1.41		0.95
sulfur dioxide	O=[S]=O	heptane	-1.36	-2.09	-3.80	-4.38
cyclodecane	C1CCCCCCCCC1	heptane	-7.11	-6.86	-12.45	-11.89
1-chlorobutane	CCCCCl	heptane	-3.96	-3.91	-7.46	-7.37
dibromomethane	BrCBr	heptane	-3.99	-4.23		-8.09
ethyl t-butyl ether	CCOC(C)(C)C	heptane	-3.98	-4.07		-7.58
methyl t-pentyl ether	CCC(C)(C)OC	heptane	-4.24	-4.17		-7.79
butanone	CCC(C)=O	heptane	-3.40	-3.55		-6.81
methyl acetate	COC(C)=O	heptane	-2.78	-3.14		-6.26
methyl hexanoate	CCCCCC(=O)OC	heptane	-5.63	-5.86		-10.52
ammonia	N	heptane	-1.27	-0.37		-1.16
n-heptylamine	CCCCCCCN	heptane	-6.17	-5.60		-10.57
n-octylamine	CCCCCCCCN	heptane	-6.88	-6.68		-12.18
dipropylamine	CCCNCCC	heptane	-4.88	-5.02	-9.12	-9.81
dibutylamine	CCCCNCCCC	heptane	-6.26	-6.20	-11.46	-11.80
piperidine	C1CCNCC1	heptane	-4.34	-5.14	-8.17	-9.60
nitromethane	C[N+](=[O-])=O	heptane	-2.62	-2.24	-5.83	-4.80
water	O	heptane	-0.59	-0.98	-2.29	-3.14
2-methylpropan-1-ol	CC(C)CO	heptane	-3.52	-3.51		-7.01
3-methylbutan-1-ol	CC(C)CCO	heptane	-3.96	-4.34		-8.37
octan-1-ol	CCCCCCCCO	heptane	-6.41	-6.53		-11.78
m-xylene	Cc1cccc(C)c1	heptane	-5.39	-5.39		-9.68
p-xylene	Cc1ccc(C)cc1	heptane	-5.39	-5.39		-9.69
ethylbenzene	CCc1ccccc1	heptane	-5.31	-5.51		-9.91
chlorobenzene	Clc1ccccc1	heptane	-5.17	-5.20		-9.36
nitrobenzene	[O-][N+](=O)c1ccccc1	heptane	-6.14	-5.57	-10.69	-9.95
deuterium	[H][H]	octane	1.34	1.45		0.98
methane	C	octane	0.16	0.11	-0.97	-1.16
2-methylpropane	CC(C)C	octane	-2.30	-2.27		-5.01
pentane	CCCCC	octane	-3.21	-3.15		-6.42
2-methylpentane	CCCC(C)C	octane	-3.71	-3.79		-7.41
3-methylheptane	CCCCC(C)CC	octane	-4.46	-5.21		-9.65
nonane	CCCCCCCCC	octane	-5.99	-6.05		-10.98
ethene	C=C	octane	-0.60	-0.71		-2.53
1,2-dichloroethane	ClCCCl	octane	-3.70	-3.78		-7.23
iodoethane	CCl	octane	-3.66	-3.77		-6.88
trifluorochloromethane	FC(F)(F)Cl	octane	-0.53	-0.66		-2.68
methyl t-butyl ether	COC(C)(C)C	octane	-3.51	-3.51		-6.91
hexan-2-one	CCCCC(C)=O	octane	-4.60	-4.97		-9.23
pentyl acetate	CCCCCOC(C)=O	octane	-5.42	-5.65		-10.33
acetone	CC(=O)C	octane	-2.17	-2.36		-4.31
2-methyl-2-butanol	CCC(C)(C)O	octane	-3.99	-3.98		-8.15
hexan-1-ol	CCCCCCO	octane	-4.99	-5.07		-9.70
3-methyl-1-pentanol	CCC(C)CCO	octane	-4.82	-4.90		-9.37
3,3-dimethyl-1-butanol	CC(C)(C)CCO	octane	-4.85	-4.68		-9.28
2-methyl-3-hexanol	CCCC(O)C(C)C	octane	-5.34	-5.33		-10.17
3-ethyl-3-pentanol	CCC(O)(CC)CC	octane	-5.42	-5.25		-10.22
2,2-dimethyl-3-pentanol	CCC(O)C(C)(C)C	octane	-4.93	-5.09		-9.94
decan-1-ol	CCCCCCCCCO	octane	-7.87	-7.98		-14.32
sulfur hexafluoride	F[S](F)(F)(F)(F)F	octane	-0.22	-0.18	-1.99	-1.70
2-furaldehyde	O=Cc1ccoc1	octane	-4.27	-4.44		-8.43
5-methylfurfural	Cc1oc(C=O)cc1	octane	-4.95	-5.45		-9.89
2-methylaniline	Cc1ccccc1N	octane	-6.34	-5.96		-10.72
argon	[Ar]	nonane	0.64	0.68	-0.35	-0.22
nitrogen	N#N	nonane	1.01	1.06		0.55

ethane	CC	nonane	-0.93	-0.66		-2.57
n-butane	CCCC	nonane	-2.47	-2.27		-5.13
2-methylpropane	CC(C)C	nonane	-2.26	-2.17		-4.95
n-heptane	CCCCCCC	nonane	-4.56	-4.60		-8.83
2,5-dimethylhexane	CC(C)CCC(C)C	nonane	-4.79	-5.11		-9.62
ethylcyclohexane	CCC1CCCCC1	nonane	-5.32	-5.46		-9.94
but-1-ene	CCC=C	nonane	-2.43	-2.22		-5.04
tetrafluoromethane	FC(F)(F)F	nonane	0.80	0.61		-0.56
furan	c1ccccc1	nonane	-2.80	-3.41		-6.92
ethyl acetate	CCOC(C)=O	nonane	-3.30	-3.62	-6.84	-7.22
butyl acetate	CCCCOC(C)=O	nonane	-4.79	-4.93		-9.29
methyl hexanoate	CCCCCC(=O)OC	nonane	-5.51	-5.75		-10.57
nitrous oxide	[O-][N+]=N	decane	-0.49	-0.05		-1.34
carbon monoxide	[C-]#[O+]	decane	0.93	0.78	0.09	-0.34
propane	CCC	decane	-1.70	-1.39	-3.28	-3.80
butane	CCCC	decane	-2.44	-2.18	-4.85	-5.04
octane	CCCCCCCC	decane	-5.16	-5.26		-10.01
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	decane	-4.82	-4.84		-9.28
methylcyclohexane	CC1CCCCC1	decane	-4.57	-4.75		-8.94
ethene	C=C	decane	-0.57	-0.53		-2.42
methyl t-pentyl ether	CCC(C)(C)OC	decane	-4.16	-4.01		-7.89
pentan-2-one	CCCC(C)=O	decane	-3.93	-4.13		-8.07
methyl acetate	COC(C)=O	decane	-2.80	-2.73		-5.80
dimethylamine	CNC	decane	-2.31	-2.31		-5.53
hexan-1-ol	CCCCCCO	decane	-4.99	-4.95		-9.70
3-methyl-1-pentanol	CCC(C)CCO	decane	-4.79	-4.78		-9.37
4,4-dimethyl-2-pentanol	CC(O)CC(C)(C)C	decane	-5.33	-4.82		-9.69
helium	[He]	undecane	2.11	1.80		1.64
xenon	[Xe]	undecane	-0.75	-0.68	-2.30	-2.55
oxygen	O=O	undecane	0.79	0.68		-0.25
carbon monoxide	[C-]#[O+]	undecane	1.02	0.79		-0.33
1,1-dichloroethane	CC(Cl)Cl	undecane	-2.86	-3.53		-7.07
1,2-dichloropropane	CC(Cl)CCl	undecane	-3.64	-4.56		-8.74
tetrachloroethene	ClC(Cl)=C(Cl)Cl	undecane	-4.41	-4.43		-8.54
bis(2-chloroethoxy)ether	C1CCOCCOCCOCC1	undecane	-8.61	-8.09		-13.42
chlorobenzene	Clc1ccccc1	undecane	-4.94	-5.14		-9.72
1,2-dichlorobenzene	Clc1ccccc1Cl	undecane	-5.93	-6.08		-11.10
neon	[Ne]	dodecane	1.95	1.66	1.67	1.29
methane	C	dodecane	0.31	0.23	-0.94	-0.97
ethylcyclohexane	CCC1CCCCC1	dodecane	-5.20	-5.46		-10.19
3-methyl-1-butene	CC(C)C=C	dodecane	-2.69	-2.69		-5.93
diethyl carbonate	CCOC(=O)OCC	dodecane	-4.41	-4.24		-8.39
1-heptanol	CCCCCCCO	dodecane	-5.35	-5.61		-10.89
2-ethyl-4-methyl-1-pentanol	CCC(CO)CC(C)C	dodecane	-5.58	-5.80		-11.30
4-ethyl-3-hexanol	CCC(O)C(CC)CC	dodecane	-5.89	-5.68		-11.16
acetophenone	CC(=O)c1ccccc1	dodecane	-5.87	-5.98		-10.81
ethyl acetate	CCOC(C)=O	dodecane	-3.30	-3.14		-6.45
isopropyl acetate	CC(C)OC(C)=O	dodecane	-3.63	-3.72		-7.42
argon	[Ar]	hexadecane	0.94	0.62	-0.19	-0.25
octane	CCCCCCCC	hexadecane	-5.02	-4.91	-9.83	-9.41
dodecane	CCCCCCCCCCCC	hexadecane	-7.77	-7.85		-14.05
cyclopropane	C1CC1	hexadecane	-1.79	-2.32		-5.05
3,3-diethylpentane	CCC(CC)(CC)CC	hexadecane	-5.21	-5.07		-9.66
ethene	C=C	hexadecane	-0.39	-0.62	-2.67	-2.43
but-1-ene	CCC=C	hexadecane	-2.03	-1.95		-4.72
oct-1-ene	CCCCCCC=C	hexadecane	-4.90	-4.92		-9.38
toluene	Cc1ccccc1	hexadecane	-4.56	-4.32	-8.58	-8.35
decan-2-one	CCCCCCCC(C)=O	hexadecane	-7.18	-7.30		-13.07
undecan-2-one	CCCCCCCCC(C)=O	hexadecane	-7.86	-7.83		-13.83
nonan-5-one	CCCCC(=O)CCCC	hexadecane	-6.33	-6.58		-11.97
3-methylbutan-2-one	CC(C)C(C)=O	hexadecane	-3.63	-3.70		-7.46
butanal	CCCC=O	hexadecane	-3.10	-3.19		-6.72
dimethyl ether	COC	hexadecane	-1.49	-1.66		-4.31
tetrahydrofuran	C1CCOC1	hexadecane	-3.46	-3.71	-6.82	-7.78
ethyl acetate	CCOC(C)=O	hexadecane	-3.24	-3.12	-6.69	-6.54
ethyl propanoate	CCOC(=O)CC	hexadecane	-3.93	-3.84		-7.67
propyl propanoate	CCCOC(=O)CC	hexadecane	-4.60	-4.52		-8.74
isobutyl formate	CC(C)COC=O	hexadecane	-3.86	-3.86		-7.68
nonan-1-ol	CCCCCCCCCO	hexadecane	-6.99	-7.05		-13.20
propan-2-ol	CC(C)O	hexadecane	-2.48	-2.43		-5.86
2-methylpropan-1-ol	CC(C)CO	hexadecane	-3.19	-3.07		-6.84
pentan-2-ol	CCCC(C)O	hexadecane	-3.87	-3.79		-8.04
2-methylbutan-2-ol	CCC(C)(C)O	hexadecane	-3.59	-3.60		-7.89
cyclopentanol	OC1CCCC1	hexadecane	-4.46	-4.90		-10.03
2,2,2-trifluoroethanol	FC(F)(F)CO	hexadecane	-1.67	-2.00	-4.99	-5.64
hexafluoropropan-2-ol	OC(F)(C(F)F)C(F)(F)F	hexadecane	-1.90	-2.47		-6.64
o-cresol	Cc1ccccc1O	hexadecane	-5.79	-5.65		-10.96
2-chlorophenol	Oc1ccccc1Cl	hexadecane	-6.73	-5.69		-10.70
3-methylbutanoic acid	CC(C)CC(=O)O	hexadecane	-4.50	-4.45		-9.35
butylamine	CCCCN	hexadecane	-3.57	-3.20	-7.03	-6.95
octylamine	CCCCCCCCN	hexadecane	-6.17	-6.04		-11.79
triethylamine	CCN(CC)CC	hexadecane	-4.20	-4.19	-8.16	-8.62
2-methylpyridine	Cc1ccccn1	hexadecane	-4.69	-4.96	-8.58	-9.22

3-methylpyridine	Cc1ccnc1	hexadecane	-4.92	-5.03	-8.96	-9.33
2,6-dimethylpyridine	Cc1cccc(C)n1	hexadecane	-5.27	-5.58		-10.23
3,4-dimethylpyridine	Cc1ccncc1C	hexadecane	-5.95	-5.67		-10.32
3,5-dimethylpyridine	Cc1cnc(C)c1	hexadecane	-5.80	-5.75		-10.50
nitrobenzene	[O-][N+](=O)c1ccccc1	hexadecane	-6.08	-5.50	-10.91	-10.56
chloroethane	CCCl	hexadecane	-2.29	-2.32		-5.39
1-chloroheptane	CCCCCCCCl	hexadecane	-5.74	-5.86		-10.93
1-chloro-2-methylpropane	CC(C)CCl	hexadecane	-3.50	-3.60		-7.41
tetrachloromethane	ClC(Cl)(Cl)Cl	hexadecane	-3.85	-4.00	-7.39	-7.57
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	hexadecane	-3.67	-4.64		-9.00
1,1,1,2-tetrachloroethane	ClCC(Cl)(Cl)Cl	hexadecane	-4.84	-5.39		-9.98
1,2-dichloropropane	CC(Cl)CCl	hexadecane	-3.89	-4.56		-8.91
1-bromohexane	CCCCCBr	hexadecane	-5.63	-5.50		-10.44
1-bromooctane	CCCCCCCBr	hexadecane	-6.94	-6.75		-12.35
2-bromobutane	CCC(C)Br	hexadecane	-4.00	-4.18		-8.42
2-bromo-2-methylpropane	CC(C)(C)Br	hexadecane	-3.57	-3.91		-8.02
dibromomethane	BrCBr	hexadecane	-3.89	-4.24		-8.70
1-iodohexane	CCCCCI	hexadecane	-6.30	-6.31		-11.11
1,1,2-trichloro-1,2,2-trifluoroethane	FC(F)(Cl)C(F)(Cl)Cl	hexadecane	-2.90	-3.30		-6.89
2-bromo-1,1,1,2-tetrafluoroethane	FC(Br)C(F)(F)F	hexadecane	-1.87	-1.81		-4.64
2-chloro-1,1,2-trifluoroethyl difluoromethyl ether	FC(F)OC(F)(F)C(F)Cl	hexadecane	-2.25	-2.69		-6.98
2,2-dichloro-1,1-difluoroethyl methyl ether	COC(F)(F)C(Cl)Cl	hexadecane	-3.91	-4.00		-8.66
tetrachloroethene	ClC(Cl)=C(Cl)Cl	hexadecane	-4.89	-4.38	-9.18	-8.43
benzyl chloride	ClCc1ccccc1	hexadecane	-5.85	-5.82	-10.35	-10.72
benzyl bromide	BrCc1ccccc1	hexadecane	-6.36	-6.30		-11.56
1,4-dichlorobenzene	Clc1ccc(Cl)cc1	hexadecane	-6.00	-6.30		-11.58
3-bromotoluene	Cc1ccccc(Br)c1	hexadecane	-6.19	-6.22		-11.47
iodobenzene	Ic1ccccc1	hexadecane	-6.25	-6.19		-10.81
ethanethiol	CCS	hexadecane	-2.96	-2.74		-5.14
diethyl disulfide	CCSSCC	hexadecane	-5.74	-5.76		-9.77
methyl <i>tert</i> -butyl ether	COC(C)(C)C	methylcyclohexane	-3.56	-3.55		-6.56
tetrahydrofuran	C1CCOC1	methylcyclohexane	-3.79	-4.07		-7.55
2,3-butanedione	CC(=O)C(C)=O	methylcyclohexane	-3.55	-4.63		-8.47
nitroethane	CC[N+](=O)[O-]	methylcyclohexane	-3.53	-3.56		-6.96
benzene	c1ccccc1	methylcyclohexane	-4.11	-4.17		-7.60
tetrafluoromethane	FC(F)(F)F	tetradecane	1.06	0.69		-0.32
ethanol	CCO	tetradecane	-1.84	-1.72		-4.58
sulfur hexafluoride	F[S](F)(F)(F)(F)F	pentadecane	0.20	-0.12		-1.59
krypton	[Kr]	cyclooctane	0.28	0.14		-0.99
sulfur hexafluoride	F[S](F)(F)(F)(F)F	cyclooctane	0.38	0.31		-1.12
nitrogen	N#N	cyclohexane	1.04	0.91	0.51	0.84
oxygen	O=O	cyclohexane	0.75	0.80	0.06	0.23
carbon monoxide	[C-]#[O+]	cyclohexane	0.89	0.65	0.20	0.02
nitric oxide	[N]=O	cyclohexane	0.47	0.32	-1.07	-0.43
propane	CCC	cyclohexane	-1.84	-1.63	-3.94	-3.49
<i>n</i> -hexane	CCCCCC	cyclohexane	-4.07	-3.88		-7.03
<i>n</i> -heptane	CCCCCCC	cyclohexane	-4.80	-4.58		-8.11
2,4-dimethylpentane	CC(C)CC(C)C	cyclohexane	-4.32	-4.33	-7.59	-7.70
1,2-dichloropropane	CC(Cl)CCl	cyclohexane	-4.27	-4.65		-8.03
2-chlorobutane	CCC(C)Cl	cyclohexane	-3.74	-3.89		-6.99
dichlorodifluoromethane	FC(F)(Cl)Cl	cyclohexane	-1.87	-1.82		-4.16
ethyl butyl ether	CCCCOCC	cyclohexane	-4.58	-4.68		-8.28
1,2-dimethoxyethane	COCOCOC	cyclohexane	-3.75	-4.14	-7.05	-7.40
dioxane	C1COCCO1	cyclohexane	-4.15	-4.53		-8.09
pentanal	CCCC=O	cyclohexane	-4.30	-4.56		-8.13
propanone	CC(C)=O	cyclohexane	-2.55	-2.92		-5.47
pentan-2-one	CCCC(C)=O	cyclohexane	-4.12	-4.43		-7.89
propyl acetate	CCCOC(C)=O	cyclohexane	-4.38	-4.71	-7.70	-8.46
methyl hexanoate	CCCCC(=O)OC	cyclohexane	-5.76	-6.11		-10.63
ethylamine	CCN	cyclohexane	-2.05	-2.50		-4.94
diethylamine	CCNCC	cyclohexane	-3.62	-3.85	-6.98	-7.57
dimethylformamide	CN(C)C=O	cyclohexane	-4.14	-4.90	-8.15	-9.31
methanol	CO	cyclohexane	-1.71	-1.64	-4.04	-3.65
pentan-2-ol	CCCC(C)O	cyclohexane	-3.86	-4.37		-8.12
hexan-2-ol	CCCCC(C)O	cyclohexane	-4.50	-5.09		-9.25
2-ethoxyethanol	CCOCCO	cyclohexane	-5.28	-4.95	-8.58	-9.42
propanethiol	CCCS	cyclohexane	-3.14	-4.10		-6.77
acetophenone	CC(=O)c1ccccc1	cyclohexane	-6.32	-6.69	-10.20	-11.39
4-methoxyaniline	COc1ccc(N)cc1	cyclohexane	-6.97	-8.35		-14.74
2,5-dimethylphenol	Cc1ccc(C)c(O)c1	cyclohexane	-6.70	-6.61		-11.38
3,5-dimethylphenol	Cc1cc(C)cc(O)c1	cyclohexane	-6.79	-6.61		-11.34
4-ethylphenol	CCc1ccc(O)cc1	cyclohexane	-6.64	-6.72		-11.51
4-propylphenol	CCCc1ccc(O)cc1	cyclohexane	-7.31	-7.44		-12.65
propane	CCC	acetone	-1.36	-1.47	-3.84	-3.37
butane	CCCC	acetone	-2.13	-2.03		-4.23
2-methylpropane	CC(C)C	acetone	-1.87	-1.90		-4.02
heptane	CCCCCCC	acetone	-3.83	-3.87	-6.40	-6.99
nonane	CCCCCCCCC	acetone	-4.99	-5.16	-8.53	-9.03
<i>trans</i> -2-butene	C/C=C/C	acetone	-2.47	-2.51		-4.96

vinylacetylene	C=CC#C	acetone	-3.19	-3.05		-5.67
chloromethane	CCl	acetone	-2.52	-2.06		-4.26
dichloromethane	ClCCl	acetone	-4.13	-3.53		-6.49
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	acetone	-4.23	-5.55		-9.71
2-chloro-2-methylpropane	CC(C)(C)Cl	acetone	-3.46	-3.54	-6.47	-6.51
1,1,2-trichlorotrifluoroethane	FC(F)(Cl)C(F)(Cl)Cl	acetone	-3.31	-3.68		-7.43
tetrahydrofuran	C1CCOC1	acetone	-4.12	-3.60	-7.72	-6.06
acetonitrile	CC#N	acetone	-3.83	-5.00	-8.01	-8.16
methylformamide	CNC=O	acetone	-7.35	-6.98	-12.17	-13.37
sulfur hexafluoride	F[S](F)(F)(F)(F)F	acetone	-0.07	0.34		-0.59
carbon disulfide	S=C=S	acetone	-3.07	-3.01	-5.78	-3.74
tetraethyllead	CC[Pb](CC)(CC)CC	acetone	-6.22	-5.59		-9.09
toluene	Cc1ccccc1	acetone	-4.98	-4.87	-8.84	-8.45
chlorobenzene	Clc1ccccc1	acetone	-5.65	-5.43		-9.22
nitrogen	N#N	methyl ethyl ketone	1.08	0.97		0.74
nitrous oxide	[O-][N+]#N	methyl ethyl ketone	-0.94	-0.92		-2.22
carbon dioxide	O=C=O	methyl ethyl ketone	-0.98	-0.74		-2.46
pentane	CCCCC	methyl ethyl ketone	-2.82	-2.72	-5.32	-5.39
heptane	CCCCCCC	methyl ethyl ketone	-4.13	-4.04	-7.45	-7.48
2,4,4-trimethylpent-1-ene	CC(=C)CC(C)(C)C	methyl ethyl ketone	-4.34	-4.12		-7.58
2,4,4-trimethylpent-2-ene	CC(C)=CC(C)(C)C	methyl ethyl ketone	-4.39	-4.04		-7.36
1-chloropropane	CCCCl	methyl ethyl ketone	-3.68	-3.37		-6.32
dimethylformamide	CN(C)C=O	methyl ethyl ketone	-6.41	-5.76		-10.56
1-hexanol	CCCCCCO	methyl ethyl ketone	-6.96	-7.02	-12.84	-13.44
3-pentanone	CCC(=O)CC	3-pentanone	-5.01	-4.80		-8.42
oxygen	O=O	2-hexanone	0.86	1.05		0.38
2-hexanone	CCCCC(C)=O	2-hexanone	-5.60	-5.33		-9.27
trichloromethane	ClC(Cl)Cl	methyl isobutyl ketone	-4.51	-4.22		-7.78
neon	[Ne]	cyclohexanone	2.26	1.94	2.10	1.86
xenon	[Xe]	cyclohexanone	-0.49	-0.49	-2.03	-2.11
nitrogen	N#N	cyclohexanone	1.44	1.01	0.65	0.34
hexane	CCCCCC	cyclohexanone	-3.33	-3.13		-6.34
heptane	CCCCCCC	cyclohexanone	-4.02	-3.86	-7.49	-7.54
2,4-dimethylpentane	CC(C)CC(C)C	cyclohexanone	-3.54	-3.44		-6.86
ethylcyclohexane	CCC1CCCCC1	cyclohexanone	-4.84	-4.78		-8.54
3-methyl-1-butene	CC(C)C=C	cyclohexanone	-2.61	-2.62		-5.38
iodomethane	CI	cyclohexanone	-3.58	-3.16		-5.95
cyclohexanone	O=C1CCCCC1	cyclohexanone	-6.34	-6.26	-10.77	-10.96
ethyl acetate	CCOC(C)=O	cyclohexanone	-4.33	-4.22		-7.56
toluene	Cc1ccccc1	cyclohexanone	-5.18	-4.70	-9.23	-8.44
triethylamine	CCN(CC)CC	cyclohexanone	-4.11	-4.32		-9.11
propane	CCC	acetophenone	-1.04	-1.30		-3.40
octane	CCCCCCCC	acetophenone	-4.26	-4.12		-7.75
2-methylpentane	CCCC(C)C	acetophenone	-2.80	-2.80		-5.64
2,5-dimethylhexane	CC(C)CCC(C)C	acetophenone	-3.75	-3.86		-7.33
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	acetophenone	-3.92	-3.55		-6.90
methylcyclohexane	CC1CCCCC1	acetophenone	-3.93	-3.81		-6.78
2-methyl-2-butene	CC=C(C)C	acetophenone	-2.79	-2.71		-5.36
pentanoic acid	CCCCC(O)=O	acetophenone	-7.78	-7.37		-14.76
heptane	CCCCCCC	cyclopentanone	-3.95	-4.01		-7.72
helium	[He]	2-methylcyclohexanone	2.35	2.07		2.22
krypton	[Kr]	2-methylcyclohexanone	0.30	0.10		-0.59
nitrogen	N#N	2-methylcyclohexanone	1.36	0.95		0.71
methane	C	2-methylcyclohexanone	0.50	-0.06		-1.16
carbon disulfide	S=C=S	benzonitrile	-3.18	-2.70		-3.58
2,4-dimethylpentane	CC(C)CC(C)C	benzonitrile	-3.23	-2.93		-5.83
cyclohexane	C1CCCCC1	benzonitrile	-3.52	-3.27		-6.02
pent-1-yne	CCCC#C	benzonitrile	-3.31	-3.30		-6.38
chloroethane	CCCl	benzonitrile	-2.88	-2.64		-5.43
propionitrile	CCC#N	benzonitrile	-4.82	-5.28		-8.55
dioxane	C1COCCO1	benzonitrile	-5.15	-5.14		-9.19
nitromethane	C[N+](=[O-])=O	benzonitrile	-4.92	-4.94		-9.29
triethylamine	CCN(CC)CC	benzonitrile	-4.06	-4.19		-9.01
sulfuryl fluoride	F[S](F)(=O)=O	tributyl phosphate	-0.65	-3.80		-7.89
hexane	CCCCCC	tributyl phosphate	-3.23	-3.20		-7.37
octane	CCCCCCCC	tributyl phosphate	-4.49	-4.43		-9.19
trans-1,2-dimethylcyclohexane	C[C@H]1CCCC[C@H]1C	tributyl phosphate	-4.49	-4.96		-9.94
cis-1,3-dimethylcyclohexane	C[C@H]1CCC[C@@H](C)C1	tributyl phosphate	-4.34	-4.99		-10.04
trans-1,3-dimethylcyclohexane	C[C@H]1CCC[C@H](C)C1	tributyl phosphate	-4.49	-4.98		-10.01
trans-1,4-dimethylcyclohexane	C[C@H]1CC[C@@H](C)CC1	tributyl phosphate	-4.43	-4.99		-10.03
1,3-butadiene	C=CC=C	tributyl phosphate	-2.29	-2.30		-6.01
1-chloropentane	CCCCCl	tributyl phosphate	-4.69	-4.60		-9.76
isopropanol	CC(C)O	tributyl phosphate	-4.73	-3.80		-9.35
carbon disulfide	S=C=S	tributyl phosphate	-3.10	-3.10		-4.01
ethylbenzene	Cc1ccccc1	tributyl phosphate	-5.40	-5.31		-10.45
m-xylene	Cc1cccc(C)c1	tributyl phosphate	-5.43	-5.23		-10.37
propylbenzene	CCCc1ccccc1	tributyl phosphate	-5.99	-5.98		-11.45
tributyl phosphate	CCCCOP(=O)(OCCCC)OCCCC	tributyl phosphate	-10.61	-8.61		-12.52
1,4-dioxane	C1COCCO1	tributyl phosphate	-4.43	-4.83		-9.93
COS	O=C=S	propylene carbonate	-1.15	-0.94		-2.50
methane	C	propylene carbonate	0.82	0.76		-1.09
butane	CCCC	propylene carbonate	-1.20	-0.91	-2.59	-3.49
hexane	CCCCCC	propylene carbonate	-2.09	-2.09	-5.02	-5.32

2,5-dimethylhexane	CC(C)CCC(C)C	propylene carbonate	-2.65	-2.73		-6.33
2-methylbut-2-ene	CC=C(C)C	propylene carbonate	-2.10	-2.04		-5.31
2-methylbuta-1,3-diene	CC(=C)C=C	propylene carbonate	-2.44	-2.56		-6.27
ethylbenzene	CCc1ccccc1	propylene carbonate	-4.82	-4.82	-9.37	-9.53
diisopropyl ether	CC(C)OC(C)C	propylene carbonate	-2.91	-3.40	-6.92	-7.39
butanone	CCC(C)=O	propylene carbonate	-4.34	-3.54		-7.51
trichloromethane	ClC(Cl)Cl	propylene carbonate	-3.93	-3.86		-8.54
t-butyl chloride	CC(C)(C)Cl	propylene carbonate	-2.77	-2.99		-6.85
krypton	[Kr]	carbon disulfide	0.20	-0.07		-1.17
deuterium	[H][H]	carbon disulfide	1.62	1.43		1.00
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	carbon disulfide	-5.00	-4.83		-8.80
methyl ethyl ketone	CCC(C)=O	carbon disulfide	-3.84	-4.51		-8.47
1-nitropropane	CCC[N+](O-)=O	carbon disulfide	-4.50	-5.35		-10.05
cyclohexane	C1CCCCC1	triethylamine	-4.18	-4.13	-7.74	-7.49
ethylcyclohexane	CCC1CCCCC1	triethylamine	-5.43	-5.44		-9.55
methyl ethyl ketone	CCC(C)=O	triethylamine	-3.69	-3.71	-7.20	-7.14
nitromethane	C[N+](O-)=O	triethylamine	-3.46	-2.77		-6.04
methyl ethyl ketone	CCC(C)=O	ethoxybenzene	-2.91	-3.98		-7.31
ethanol	CCO	ethoxybenzene	-4.63	-3.84		-8.47
nitromethane	C[N+](O-)=O	ethoxybenzene	-4.33	-4.46		-8.88
ethanol	CCO	2-methylpyridine	-4.94	-4.39		-9.40
1-propanol	CCCO	2-methylpyridine	-5.54	-5.03		-10.39
1-butanol	CCCCO	2-methylpyridine	-6.18	-5.62		-11.29
toluene	Cc1ccccc1	2-methylpyridine	-5.18	-5.19		-9.09
methane	C	anisole	0.61	0.14		-0.89
nonane	CCCCCCCCC	anisole	-5.34	-5.55		-9.78
2-methylpentane	CCCC(C)C	anisole	-3.16	-3.23		-6.04
2,5-dimethylhexane	CC(C)CCC(C)C	anisole	-4.19	-4.63		-8.38
ethylcyclohexane	CCC1CCCCC1	anisole	-4.89	-5.01		-8.43
nitromethane	C[N+](O-)=O	benzyl ether	-4.35	-4.92		-10.22
methyl ethyl ketone	CCC(C)=O	3-methylphenol	-6.03	-4.16		-7.84
xenon	[Xe]	acetic acid	-0.29	-0.14	-1.37	-1.85
oxygen	O=O	acetic acid	0.97	0.17		-2.31
nitrous oxide	[O-][N+]#N	acetic acid	-0.90	-0.46		-2.17
carbon monoxide	[C-]#[O+]	acetic acid	1.05	0.99	0.31	-0.33
octane	CCCCCCCC	acetic acid	-4.01	-4.36	-8.19	-8.51
isooctane	CCCCCC(C)C	acetic acid	-3.09	-4.40		-8.61
cyclopropane	C1CC1	acetic acid	-1.67	-1.39		-3.43
2-methyl-1-propene	CC(C)=C	acetic acid	-2.10	-1.75		-4.35
nitromethane	C[N+](O-)=O	acetic acid	-4.84	-4.06		-8.29
2-chloro-2-methylpropane	CC(C)(C)Cl	acetic acid	-3.06	-3.33	-6.55	-6.87
methyl ethyl ketone	CCC(C)=O	nitroethane	-4.79	-4.19		-7.75
2,4-dimethylpentane	CC(C)CC(C)C	benzyl alcohol	-2.77	-3.24		-6.77
toluene	Cc1ccccc1	benzyl alcohol	-4.59	-4.71		-8.81
hexane	CCCCCC	butyronitrile	-3.18	-3.07		-6.39
2-methylpentane	CCCC(C)C	butyronitrile	-3.01	-2.88		-6.08
2,5-dimethylhexane	CC(C)CCC(C)C	butyronitrile	-3.97	-4.11		-8.08
1-hexene	CCCCC=C	butyronitrile	-3.34	-3.43		-6.87
1-octene	CCCCCCC=C	butyronitrile	-4.52	-4.81		-9.12
butan-1-ol	CCCCO	butyronitrile	-5.39	-5.51		-11.76
2-methylpropan-1-ol	CC(C)CO	butyronitrile	-5.20	-5.27		-11.38
2-methylpropan-2-ol	CC(C)(C)O	butyronitrile	-4.42	-4.51		-10.09
octan-1-ol	CCCCCCCCO	butyronitrile	-7.87	-8.30		-16.25
nitrogen	N#N	aniline	1.97	0.94		-0.16
nitrous oxide	[O-][N+]#N	aniline	-0.20	-1.26		-3.61
carbon monoxide	[C-]#[O+]	aniline	1.74	0.73		-0.82
hydrogen sulfide	S	aniline	-1.70	-1.97		-3.97
1-pentene	CCCC=C	aniline	-2.06	-2.67		-5.79
1-heptene	CCCCCC=C	aniline	-3.24	-4.00		-7.91
2-methyl-2-pentene	CCC=C(C)C	aniline	-2.79	-3.25		-6.71
trichloromethane	ClC(Cl)Cl	aniline	-3.88	-4.28		-8.53
chloroethane	CCCl	aniline	-2.65	-2.42		-5.39
methyl iodide	CI	aniline	-3.07	-3.24		-6.60
acetonitrile	CC#N	aniline	-4.68	-3.95		-6.73
2-methylpentane	CCCC(C)C	nitromethane	-2.15	-2.27	-3.82	-4.43
cyclohexane	C1CCCCC1	nitromethane	-2.71	-2.78	-4.64	-4.77
acetone	CC(C)=O	nitromethane	-4.33	-3.73		-7.10
ethanol	CCO	nitromethane	-3.88	-3.94	-7.26	-8.70
hexane	CCCCCC	nitrobenzene	-2.95	-2.66		-5.15
nonane	CCCCCCCCC	nitrobenzene	-4.82	-4.17		-7.39
trimethylamine	CN(C)C	nitrobenzene	-3.92	-2.82		-5.93
neon	[Ne]	dimethyl sulfoxide	2.59	1.71		1.29
argon	[Ar]	dimethyl sulfoxide	1.74	1.22		0.34
krypton	[Kr]	dimethyl sulfoxide	1.11	0.98		-0.61
hydrogen	[H][H]	dimethyl sulfoxide	2.16	1.67		1.00
pentane	CCCCC	dimethyl sulfoxide	-1.47	-1.24	-3.64	-4.20
2-methylpentane	CCCC(C)C	dimethyl sulfoxide	-1.79	-1.62		-4.79
2,3,4-trimethylpentane	CC(C)C(C)C(C)C	dimethyl sulfoxide	-2.60	-2.01		-5.43
dichloromethane	ClCCl	dimethyl sulfoxide	-4.11	-2.58	-8.19	-6.49
chloroform	ClC(Cl)Cl	dimethyl sulfoxide	-4.75	-3.39	-8.79	-7.88
ethyl tert-butyl ether	CCOC(C)(C)C	dimethyl sulfoxide	-2.69	-3.06	-6.57	-7.17
acetonitrile	CC#N	dimethyl sulfoxide	-4.59	-3.69	-7.94	-7.06
nonane	CCCCCCCCC	propionitrile	-4.69	-5.01		-9.38

ethylcyclohexane	CCC1CCCCC1	propionitrile	-4.32	-4.59		-8.29
dichloromethane	ClCCl	propionitrile	-3.91	-3.27		-6.32
triethylamine	CCN(CC)CC	propionitrile	-4.02	-4.17		-8.91
sulfur dioxide	O=[S]=O	acetonitrile	-3.33	-2.69	-7.10	-6.40
2,2-dimethylbutane	CCC(C)(C)C	acetonitrile	-2.39	-2.40		-5.16
2,3,4-trimethylpentane	CC(C)(C)C(C)C	acetonitrile	-3.42	-3.26		-6.44
1-hexene	CCCCC=C	acetonitrile	-2.97	-3.27		-6.32
ethyl acetate	CCOC(C)=O	acetonitrile	-4.61	-4.50		-7.90
water	O	acetonitrile	-4.44	-4.13	-8.63	-10.12
octane	CCCCCCCC	ethyl benzoate	-4.64	-4.32		-7.78
methylcyclohexane	CC1CCCCC1	ethyl benzoate	-4.16	-4.24		-7.56
diethyl ether	CCOCC	ethyl benzoate	-3.10	-3.42		-6.57
nitrous oxide	[O-][N+]=N	sulfolane	-0.47	-0.16		-3.07
butane	CCCC	sulfolane	-0.80	-0.79		-4.26
heptane	CCCCCCC	sulfolane	-2.48	-2.52		-6.95
methylcyclohexane	CC1CCCCC1	sulfolane	-2.70	-3.11		-7.87
isobutene	CC(C)=C	sulfolane	-1.27	-1.16		-4.84
1,3-butadiene	C=CC=C	sulfolane	-1.81	-1.67		-5.64
1-hexene	CCCCC=C	sulfolane	-2.08	-2.33		-6.54
chloroethane	CCCl	sulfolane	-2.44	-1.82		-5.97
diethyl ether	CCOCC	sulfolane	-2.37	-2.66		-7.13
tetrahydrofuran	C1CCOC1	sulfolane	-3.70	-3.25		-8.04
dioxane	C1COCCO1	sulfolane	-4.70	-4.45		-10.03
acetone	CC(C)=O	sulfolane	-3.70	-2.79		-7.27
methanol	CO	sulfolane	-3.82	-3.26		-10.00
ethanol	CCO	sulfolane	-4.06	-3.74		-10.83
butan-1-ol	CCCCO	sulfolane	-5.06	-4.65		-12.21
allyl alcohol	OCC=C	sulfolane	-5.04	-5.12		-13.12
benzene	c1ccccc1	sulfolane	-4.01	-3.26		-7.86
m-xylene	Cc1cccc(C)c1	sulfolane	-4.86	-4.38		-9.59
nitrogen	N#N	pyridine	1.53	0.93		0.65
octane	CCCCCCCC	pyridine	-4.48	-4.67		-8.40
cyclohexane	C1CCCCC1	pyridine	-3.71	-3.58		-6.01
ethylcyclohexane	CCC1CCCCC1	pyridine	-4.74	-4.83		-8.03
trichloromethane	ClC(Cl)Cl	pyridine	-4.63	-4.69	-9.18	-8.49
1-chlorobutane	CCCCCl	pyridine	-4.33	-4.31	-7.60	-7.73
tetrahydrofuran	C1CCOC1	pyridine	-4.34	-3.86		-6.56
butanone	CCC(C)=O	pyridine	-4.66	-4.65	-8.29	-8.21
2-methyl-isopropanol	CC(C)(C)O	pyridine	-5.07	-4.61		-9.53
toluene	Cc1ccccc1	pyridine	-5.12	-5.21	-9.08	-9.04
bromobenzene	BrC1ccccc1	pyridine	-6.34	-6.14	-10.37	-10.40
iodobenzene	Ic1ccccc1	pyridine	-7.37	-7.09	-11.38	-11.56
hydrogen	[H][H]	diethyl carbonate	1.51	0.49		-0.61
carbon dioxide	O=C=O	diethyl carbonate	-0.97	-0.46	-2.85	-2.68
methane	C	diethyl carbonate	0.36	0.37	-0.43	-0.55
ethene	C=C	diethyl carbonate	-0.68	-0.78	-1.99	-2.70
octane	CCCCCCCC	diethyl carbonate	-4.69	-4.70		-8.58
decane	CCCCCCCCC	2-butanol		-6.21	-11.21	-11.41
3-ethylpentane	CCC(CC)CC	2-butanol		-3.88	-7.73	-7.66
ethene	C=C	2-butanol		-0.96	-2.33	-2.90
1-butene	CCC=C	2-butanol		-2.30	-4.88	-4.95
1-heptene	CCCCC=C	2-butanol		-4.41	-7.77	-8.38
2,4,4-trimethyl-1-pentene	CC(=C)CC(C)(C)C	2-butanol		-4.11	-7.78	-7.92
1,3-butadiene	C=CC=C	2-butanol		-2.60	-4.84	-5.32
chloroethane	CCCl	2-butanol		-2.58	-4.89	-5.27
1-chlorobutane	CCCCCl	2-butanol		-3.91	-6.97	-7.32
2-chloro-2-methylpropane	CC(C)(C)Cl	2-butanol		-3.28	-5.71	-6.16
2-methyl-2-bromopropane	CC(C)(C)Br	2-butanol		-3.65	-6.41	-6.94
acetone	CC(C)=O	2-butanol		-3.21	-5.38	-5.78
helium	[He]	2-butanol		2.06	1.95	2.10
nitrogen	N#N	2-butanol		0.98	0.10	0.40
oxygen	O=O	2-butanol		1.04	-0.34	0.16
carbon tetrafluoride	FC(F)(F)F	2-butanol		0.88	-0.53	-0.51
hydrogen sulfide	S	2-butanol		-1.55	-2.57	-2.55
methyl propionate	CCC(=O)OC	2-butanol		-3.80	-6.53	-6.58
tetramethylsilane	C[Si](C)(C)C	2-butanol		-2.87	-5.16	-5.34
ethylene carbonate	O=C1OCCO1	2-butanol		-5.21	-7.29	-9.23
benzamide	NC(=O)c1ccccc1	2-butanol		-10.92	-18.44	-19.26
benzoic acid	OC(=O)c1ccccc1	2-butanol		-9.54	-16.92	-17.64
isobutane	CC(C)C	isobutanol		-1.70	-5.01	-4.19
butane	CCCC	isobutanol		-1.86	-5.20	-4.46
nonane	CCCCCCCCC	isobutanol		-5.48	-10.42	-10.37
tetradecane	CCCCCCCCCCCCC	isobutanol		-8.86	-15.82	-15.97
bicyclohexyl	C1CCC(CC1)C2CCCCC2	isobutanol		-7.64	-13.18	-12.72
1-propene	CC=C	isobutanol		-1.53	-4.27	-3.84
1-heptene	CCCCC=C	isobutanol		-4.33	-8.07	-8.36
decan-1-ol	CCCCCCCCCO	isobutanol		-9.63	-19.09	-18.37
2-butanol	CCC(C)O	isobutanol		-5.27	-11.88	-11.25
1-chlorobutane	CCCCCl	isobutanol		-3.91	-7.16	-7.45
2-methyl-2-bromobutane	CCC(C)(C)Br	isobutanol		-4.20	-8.12	-7.99
1-bromoadamantane	BrC12CC3CC(C(C3)C1)C2	isobutanol		-8.01	-13.15	-13.10
dimethyl ether	COC	isobutanol		-2.05	-4.33	-4.27
helium	[He]	isobutanol		2.04	1.47	2.07



neon	[Ne]	isobutanol		1.87	1.17	1.72
deuterium	[H][H]	isobutanol		1.53	0.83	1.01
butyl formate	CCCCOC=O	isobutanol		-4.65	-8.08	-8.29
triethylamine	CCN(CC)CC	isobutanol		-4.42	-10.55	-9.39
ethylene carbonate	O=C1OCCO1	isobutanol		-5.12	-7.82	-9.17
benzamide	NC(=O)c1ccccc1	isobutanol		-10.88	-18.79	-19.19
butane	CCCC	1-propanol		-1.78	-5.28	-4.35
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	1-propanol		-3.72	-7.98	-7.65
1-butene	CCC=C	1-propanol		-2.19	-4.73	-4.93
1,3-butadiene	C=CC=C	1-propanol		-2.50	-5.00	-5.31
hexan-1-ol	CCCCCCO	1-propanol		-6.92	-14.46	-14.11
decan-1-ol	CCCCCCCCCO	1-propanol		-9.61	-19.12	-18.43
2-methyl-2-bromopropane	CC(C)(C)Br	1-propanol		-3.60	-7.12	-7.04
dibutyl ether	CCCCOCCCC	1-propanol		-5.79	-10.31	-10.57
n-butyl methyl ether	CCCCOC	1-propanol		-3.79	-7.43	-7.16
3,6,9-trioxundecane	CCC(=O)CCC(=O)CCC(=O)CC	1-propanol		-9.65	-12.28	-15.17
pentaglyme	COCOCOCOCOCOCOC	1-propanol		-12.32		-21.80
benzo-15-crown-5	C1COCCOCc2ccccc2OCCOCCO1	1-propanol		-13.98	-19.70	-26.41
propyl acetate	CCCOC(C)=O	1-propanol		-4.53	-8.08	-8.11
methyl lactate	COC(=O)C(C)O	1-propanol		-6.70	-11.76	-13.76
nitromethane	C[N+](=[O-])=O	1-propanol		-4.30	-7.09	-8.11
tributylamine	CCCCN(CCCC)CCCC	1-propanol		-7.58	-15.82	-15.18
formamide	NC=O	1-propanol		-7.07	-13.58	-14.04
ethylene carbonate	O=C1OCCO1	1-propanol		-5.15	-7.58	-9.28
benzaldehyde	O=Cc1ccccc1	1-propanol		-6.54	-10.55	-10.91
quinoline	c1ccc2ncccc2c1	1-propanol		-9.19	-14.02	-15.09
difluoromethane	FCF	1-propanol		-1.05	-2.25	-2.55
carbon dioxide	O=C=O	1-pentanol		-0.28	-2.22	-2.44
ethane	CC	1-pentanol		-0.31	-2.39	-2.17
decane	CCCCCCCCC	1-pentanol		-6.14	-11.77	-11.61
dodecane	CCCCCCCCCCCC	1-pentanol		-7.46	-14.09	-13.88
methylcyclohexane	CC1CCCCC1	1-pentanol		-4.43	-7.96	-8.55
bicyclohexyl	C1CCC(CC1)C2CCCCC2	1-pentanol		-7.82	-13.40	-13.36
cis-2-butene	C/C=C/C	1-pentanol		-2.03	-5.17	-4.73
1-heptene	CCCCCC=C	1-pentanol		-4.24	-8.24	-8.41
methanol	CO	1-pentanol		-3.54	-8.37	-8.52
pentan-1-ol	CCCCCO	1-pentanol		-6.33	-13.60	-13.33
nonan-1-ol	CCCCCCCCCO	1-pentanol		-9.04	-18.27	-17.63
diethyl ether	CCOCC	1-pentanol		-3.01	-6.31	-5.98
dichloromethane	CICCl	1-pentanol		-3.05	-6.21	-6.21
2-chloro-2-methylbutane	CCC(C)(C)Cl	1-pentanol		-3.95	-7.67	-7.59
2-chloro-2-methylpentane	CCCC(C)(C)Cl	1-pentanol		-4.56	-8.91	-8.59
1,5-dichloropentane	C1CCCCC1	1-pentanol		-6.48	-10.99	-11.29
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	1-pentanol		-6.59	-11.31	-11.77
dimethylformamide	CN(C)C=O	1-pentanol		-5.39	-9.99	-10.44
d-limonene	CC(=C)C1CCC(=CC1)C	1-pentanol		-6.73	-11.24	-12.14
1,1,2-trifluorotrichloroethane	FC(F)(Cl)C(F)(Cl)Cl	1-pentanol		-3.21	-5.79	-7.27
ethane	CC	1-butanol		-0.36	-2.90	-2.20
propane	CCC	1-butanol		-1.09	-4.23	-3.33
cyclopentane	C1CCCC1	1-butanol		-3.10	-7.30	-6.27
cyclohexane	C1CCCCC1	1-butanol		-3.88	-7.55	-7.58
methylcyclohexane	CC1CCCCC1	1-butanol		-4.40	-7.88	-8.41
ethene	C=C	1-butanol		-0.80	-2.49	-2.85
1-hexene	CCCCC=C	1-butanol		-3.50	-6.22	-7.11
1-heptene	CCCCCC=C	1-butanol		-4.21	-8.22	-8.28
acetylene	C#C	1-butanol		-1.32	-3.58	-3.76
pentan-1-ol	CCCCCO	1-butanol		-6.35	-13.55	-13.28
octan-1-ol	CCCCCCCCO	1-butanol		-8.40	-16.79	-16.54
decan-1-ol	CCCCCCCCCO	1-butanol		-9.64	-19.23	-18.58
dibutyl ether	CCCCOCCCC	1-butanol		-5.79	-10.16	-10.64
15-crown-5	C1COCCOCCOCCOCCO1	1-butanol		-10.34	-16.82	-20.08
1-bromobutane	CCCCBr	1-butanol		-4.24	-8.15	-8.23
2-methyl-2-iodopropane	CC(C)(C)I	1-butanol		-4.24	-7.86	-7.51
xenon	[Xe]	1-butanol		-0.56	-2.51	-2.37
carbon monoxide	C=O	1-butanol		0.87	-0.34	-0.27
carbon dioxide	O=C=O	1-butanol		-0.48	-2.73	-2.74
carbon tetrafluoride	FC(F)(F)F	1-butanol		0.97	-0.41	-0.57
propyl formate	CCCOC=O	1-butanol		-3.78	-7.49	-6.86
methyl butanoate	CCCC(=O)OC	1-butanol		-4.39	-7.98	-7.86
methyl pentanoate	CCCCC(=O)OC	1-butanol		-4.99	-8.84	-8.83
methyl undecanoate	CCCCCCCCCCC(=O)OC	1-butanol		-9.08	-15.48	-15.87
ethyl hexanoate	CCCCCC(=O)OCC	1-butanol		-6.33	-10.99	-11.20
ethyl lactate	CCOC(=O)C(C)O	1-butanol		-6.73	-12.10	-13.96
ethylbenzene	CCc1ccccc1	1-butanol		-5.38	-9.59	-9.72
ethylene carbonate	O=C1OCCO1	1-butanol		-5.05	-8.10	-9.19
2-pyrrolidone	O=C1CCCN1	1-butanol		-8.67	-16.08	-16.08
N-methylimidazole	Cn1ccnc1	1-butanol		-6.88	-13.50	-11.67
2-methylpentane	CCCC(C)C	1-hexanol		-3.11	-6.90	-6.75
1-heptene	CCCCC=C	1-hexanol		-4.25	-8.26	-8.48
propan-1-ol	CCCO	1-hexanol		-4.89	-11.25	-10.98
butan-1-ol	CCCCO	1-hexanol		-5.45	-12.43	-11.87
dipropyl ether	CCOCCC	1-hexanol		-4.28	-8.03	-8.19
1-chlorooctane	CCCCCCCCCl	1-hexanol		-6.46	-11.92	-11.86

1,2-dichloropropane	CC(Cl)CCl	1-hexanol	-4.82	-7.79	-8.79
1,3-dichloropropane	ClCCCCl	1-hexanol	-4.81	-8.71	-8.85
1,4-dichlorobutane	ClCCCCl	1-hexanol	-5.63	-9.95	-9.96
acetone	CC(C)=O	1-hexanol	-2.72	-5.62	-5.24
2-hexanone	CCCCC(C)=O	1-hexanol	-5.04	-8.41	-9.12
dimethyl sulfoxide	C[S](C)=O	1-hexanol	-6.72	-11.38	-11.98
1-heptylamine	CCCCCCCN	1-hexanol	-6.77	-14.32	-14.26
<i>n</i> -ethyl- <i>n</i> -butylamine	CCCCNCC	1-hexanol	-5.72	-12.28	-12.61
tributylamine	CCCCN(CCCC)CCCC	1-hexanol	-7.74	-15.80	-15.66
bromobenzene	BrCc1ccccc1	1-hexanol	-5.66	-10.20	-10.21
chlorobenzene	Clc1ccccc1	1-hexanol	-5.25	-9.29	-9.53
quinoline	c1ccc2ncccc2c1	1-hexanol	-8.90	-14.09	-14.82
butane	CCCC	isopropanol	-1.92	-4.63	-4.43
3,3-dimethylpentane	CCC(C)(C)CC	isopropanol	-3.34	-7.44	-6.80
<i>trans</i> -2-butene	C/C=C\C	isopropanol	-2.30	-5.16	-4.91
2,4,4-trimethyl-1-pentene	CC(=C)CC(C)(C)C	isopropanol	-4.07	-7.93	-7.85
pentan-1-ol	CCCCCO	isopropanol	-6.44	-13.56	-13.11
2-chloro-2-methylpentane	CCCC(C)(C)Cl	isopropanol	-4.60	-8.56	-8.30
2-methyl-2-bromobutane	CCC(C)(C)Br	isopropanol	-4.16	-8.03	-7.75
2-methyl-2-iodopropane	CC(C)(C)I	isopropanol	-4.20	-7.42	-7.13
argon	[Ar]	isopropanol	0.89	-0.89	0.11
methyl propionate	CCC(=O)OC	isopropanol	-3.95	-6.69	-6.83
sec-butylamine	CCC(C)N	isopropanol	-4.25	-9.38	-9.77
dibutylamine	CCCCNCCCC	isopropanol	-6.39	-13.65	-13.52
succinic acid	OC(=O)CCC(O)=O	isopropanol	-11.37	-22.45	-22.81
1,3-diaminopropane	NCCCN	isopropanol	-7.24	-15.00	-15.63
anthracene	c1ccc2cc3ccccc3cc2c1	isopropanol	-10.56	-16.06	-17.37
<i>n</i> -methylpyrrole	Cn1cccc1	isopropanol	-5.31	-8.36	-9.72
difluoromethane	FCF	isopropanol	-1.16	-2.80	-2.58
water	O	isopropanol	-4.04	-10.13	-9.88
decane	CCCCCCCCC	tetrahydrofuran	-6.42	-11.03	-11.01
ethene	C=C	tetrahydrofuran	-1.46	-2.73	-3.44
cyclohexene	C1CCC=CC1	tetrahydrofuran	-4.35	-7.73	-7.54
dichloromethane	ClCCl	tetrahydrofuran	-3.86	-8.17	-7.18
1-chlorobutane	CCCCCl	tetrahydrofuran	-4.30	-8.24	-7.83
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	tetrahydrofuran	-7.19	-13.63	-12.36
methyl benzoate	COC(=O)c1ccccc1	tetrahydrofuran	-8.26	-13.70	-13.90
propyl benzoate	CCCOC(=O)c1ccccc1	tetrahydrofuran	-9.27	-15.73	-15.41
1-butanol	CCCCO	tetrahydrofuran	-5.90	-11.44	-11.69
1-hexanol	CCCCCCO	tetrahydrofuran	-7.22	-13.62	-13.65
1-nonanol	CCCCCCCCCO	tetrahydrofuran	-9.02	-17.01	-16.29
butyronitrile	CCCC#N	tetrahydrofuran	-5.54	-9.48	-8.69
toluene	Cc1ccccc1	tetrahydrofuran	-5.42	-9.27	-9.51
1,2,4-trimethylbenzene	Cc1ccc(C)c(C)c1	tetrahydrofuran	-6.61	-11.64	-11.41
nitrobenzene	[O-][N+](=O)c1ccccc1	tetrahydrofuran	-7.74	-13.80	-13.43
krypton	[Kr]	tetrahydrofuran	0.08	-0.81	-0.62
xenon	[Xe]	tetrahydrofuran	-0.97	-2.12	-2.31
carbon tetrafluoride	FC(F)(F)F	tetrahydrofuran	0.93	0.00	0.26
2-methylpyridine	Cc1cccn1	tetrahydrofuran	-6.76	-10.04	-11.12
4-methylpyridine	Cc1ccncc1	tetrahydrofuran	-6.75	-10.59	-11.03
dimethyl carbonate	COC(=O)OC	tetrahydrofuran	-4.73	-8.82	-8.17
butylamine	CCCCN	tetrahydrofuran	-5.19	-8.24	-10.01
methylformamide	CNC=O	tetrahydrofuran	-7.24	-12.12	-13.86
acetamide	CC(N)=O	tetrahydrofuran	-7.78	-14.76	-15.11
<i>n</i> -methylacetamide	CNC(C)=O	tetrahydrofuran	-7.69	-15.36	-14.59
4-methoxyphenol	COc1ccc(O)cc1	tetrahydrofuran	-10.11	-19.48	-18.61
4-chlorophenol	Oc1ccc(Cl)cc1	tetrahydrofuran	-9.50	-19.10	-17.45
2,4,6-trimethylphenol	Cc1cc(C)c(O)c(C)c1	tetrahydrofuran	-9.57	-18.14	-17.36
2,4-di- <i>tert</i> -butylphenol	CC(C)(C)c1ccc(O)c(c1)C(C)(C)C	tetrahydrofuran	-10.90	-22.13	-19.23
3,5-dimethyl-1 <i>H</i> -pyrazole	Cc1[nH]nc(C)c1	tetrahydrofuran	-8.57	-15.68	-15.42
1,2,3-benzotriazole	[nH]1nnc2ccccc12	tetrahydrofuran	-9.20		-15.16
δ-valerolactam	O=C1CCCCN1	tetrahydrofuran	-9.07	-15.46	-16.32
nitrogen	N#N	dichloromethane	0.87	1.41	0.64
iodine	I2	dichloromethane	-5.66	-9.07	-9.28
cyclohexane	C1CCCCC1	dichloromethane	-4.18	-6.44	-7.42
1-chlorobutane	CCCCCl	dichloromethane	-4.49	-7.83	-8.18
1,4-dichlorobutane	ClCCCCCl	dichloromethane	-6.43	-11.34	-10.93
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	dichloromethane	-6.59	-11.04	-11.01
2-chloro-2-methylpropane	CC(C)(C)Cl	dichloromethane	-4.08	-6.74	-7.52
2-bromo-2-methylpropane	CC(C)(C)Br	dichloromethane	-4.08	-7.44	-7.52
tetrahydrofuran	C1CCOC1	dichloromethane	-4.79	-8.71	-8.59
butanone	CCC(C)=O	dichloromethane	-4.92	-9.08	-8.73
propyl acetate	CCCOC(C)=O	dichloromethane	-5.92	-9.55	-10.49
acetonitrile	CC#N	dichloromethane	-5.14	-8.57	-8.38
butyronitrile	CCCC#N	dichloromethane	-6.27	-10.13	-10.18
nitroethane	CC[N+](=O)[O-]	dichloromethane	-5.69	-9.77	-10.27
methanol	CO	dichloromethane	-3.12	-6.17	-6.48
ethanol	CCO	dichloromethane	-3.84	-7.07	-7.78
methylformamide	CNC=O	dichloromethane	-6.81	-11.84	-12.72
<i>n</i> -methylacetamide	CNC(C)=O	dichloromethane	-7.71	-12.97	-14.64
1,4-diphenylbenzene	c1ccc(cc1)c2ccc(cc2)c3ccccc3	dichloromethane	-13.79	-21.56	-21.99
chlorobenzene	Clc1ccccc1	dichloromethane	-5.83	-9.52	-9.96
piperidine	C1CCNCC1	dichloromethane	-6.42	-9.70	-11.93

2-methylpyridine	Cc1ccccn1	dichloromethane		-7.36	-11.04	-12.41
phenyl benzoate	O=C(Oc1ccccc1)c2ccccc2	dichloromethane		-12.22	-18.42	-19.71
2-nitrophenol	Oc1ccccc1[N+](=O)[O-]	dichloromethane		-8.54	-13.59	-14.78
propane	CCC	methanol		-0.98	-3.13	-2.89
3,3-diethylpentane	CCC(CC)(CC)CC	methanol		-4.25	-8.90	-8.49
2,2,4-trimethylpentane	CC(C)CC(C)(C)C	methanol		-3.50	-7.04	-7.20
2,2,4,4-tetramethylpentane	CC(C)(C)CC(C)(C)C	methanol		-3.69	-7.72	-7.64
2,2,5,5-tetramethylhexane	CC(C)(C)CCC(C)(C)C	methanol		-4.38	-8.20	-8.76
cyclohexane	C1CCCCC1	methanol		-3.47	-6.72	-6.63
methylcyclohexane	CC1CCCCC1	methanol		-3.95	-7.24	-7.39
1-decene	CCCCCCCC=C	methanol		-5.73	-10.58	-10.41
cis-4-octene	CCC/C=C/CCC	methanol		-4.44	-8.29	-8.32
cyclohexene	C1CCC=CC1	methanol		-3.78	-7.06	-7.10
1-methylcyclohexene	CC1=CCCCC1	methanol		-4.21	-8.09	-7.75
cycloheptene	C1CCC=CCC1	methanol		-4.35	-7.75	-8.00
propan-1-ol	CCCO	methanol		-4.83	-10.96	-10.46
pentan-1-ol	CCCCCO	methanol		-6.10	-13.22	-12.60
hexan-1-ol	CCCCCCO	methanol		-6.66	-14.23	-13.53
undecan-1-ol	CCCCCCCCCO	methanol		-9.94	-19.02	-18.80
1,3-propanediol	OCCO	methanol		-7.72	-17.09	-16.79
glycerol	OCC(O)CO	methanol		-6.58	-21.53	-16.01
ethylbenzene	CCc1ccccc1	methanol		-5.30	-9.55	-9.45
tert-butylbenzene	CC(C)(C)c1ccccc1	methanol		-6.25	-10.67	-11.11
tetrachloromethane	ClC(Cl)(Cl)Cl	methanol		-4.21	-7.88	-8.10
chloroethane	CCCl	methanol		-2.56	-5.67	-5.31
methyl iodide	CI	methanol		-3.24	-6.20	-6.03
acetone	CC(C)=O	methanol		-3.68	-6.88	-6.82
3-pentanone	CCC(=O)CC	methanol		-4.83	-8.61	-8.59
6-undecanone	CCCCC(=O)CCCCC	methanol		-8.35	-13.73	-14.69
tert-butyl methyl ketone	CC(=O)C(C)(C)C	methanol		-4.77	-8.49	-8.64
dimethyl ether	COC	methanol		-2.08	-4.23	-4.26
15-crown-5	C1COCCOCCOCCOCCO1	methanol		-10.70	-21.82	-20.71
carbon monoxide	C=O	methanol		0.45	0.16	-0.77
propyl acetate	CCCOC(C)=O	methanol		-4.86	-8.54	-8.64
butyronitrile	CCCC#N	methanol		-5.80	-8.57	-9.48
dimethyl sulfoxide	C[S](C)=O	methanol		-7.10	-12.88	-12.27
diethylamine	CCNCC	methanol		-4.47	-11.71	-10.13
4-methylphenol	Cc1ccc(O)cc1	methanol		-8.16	-15.93	-15.12
4-methylpyridine	Cc1ccncc1	methanol		-6.29	-12.05	-10.47
3,5-dimethylpyridine	Cc1cnc(C)c1	methanol		-7.08	-13.09	-11.96
methyl benzoate	COC(=O)c1ccccc1	methanol		-7.40	-12.19	-12.22
nitrobenzene	[O-][N+](=O)c1ccccc1	methanol		-7.43	-12.15	-12.48
1-chloro-3-nitrobenzene	[O-][N+](=O)c1ccc(Cl)cc1	methanol		-8.64	-13.83	-14.43
styrene	C=Cc1ccccc1	methanol		-5.55	-10.05	-9.77
trifluorotoluene	Cc1ccc(F)c(F)c1F	methanol		-5.20	-9.03	-9.39
methylformamide	CNC=O	methanol		-6.88	-12.69	-13.26
propane	CCC	ethanol		-1.10	-3.36	-3.20
isobutane	CC(C)C	ethanol		-1.59	-4.80	-3.96
hexane	CCCCCC	ethanol		-3.04	-6.89	-6.27
nonane	CCCCCCCCC	ethanol		-5.13	-10.13	-9.67
hexadecane	CCCCCCCCCCCCCCCC	ethanol		-9.79	-17.59	-17.28
cyclohexane	C1CCCCC1	ethanol		-3.69	-7.23	-7.06
bicyclohexyl	C1CCC(CC1)C2CCCCC2	ethanol		-7.51	-12.88	-12.53
4-octyne	CCCC#CCCC	ethanol		-4.95	-9.58	-9.07
propan-1-ol	CCCO	ethanol		-4.90	-11.04	-10.63
pentan-1-ol	CCCCCO	ethanol		-6.29	-13.30	-12.99
octan-1-ol	CCCCCCCCO	ethanol		-8.32	-16.58	-16.22
ethylene glycol	OCCO	ethanol		-6.22	-15.14	-14.57
1,2-propanediol	CC(O)CO	ethanol		-6.72	-16.69	-15.61
methyl tert-butyl ether	COC(C)(C)C	ethanol		-3.43	-7.02	-6.74
1,4-dioxane	C1COCCO1	ethanol		-4.81	-7.88	-8.65
1,2-dimethoxyethane	COCCOC	ethanol		-4.80	-8.30	-8.70
2-methyl-2-bromopropane	CC(C)(C)Br	ethanol		-3.54	-7.18	-6.85
2-methyl-2-chloropropane	CC(C)(C)Cl	ethanol		-3.34	-6.57	-6.41
2-methyl-2-iodopropane	CC(C)(C)I	ethanol		-4.42	-8.03	-7.70
α-methylstyrene	CC(=C)c1ccccc1	ethanol		-6.12	-11.26	-10.70
acetone	CC(C)=O	ethanol		-3.52	-6.26	-6.53
methyl ethyl ketone	CCC(C)=O	ethanol		-4.14	-7.37	-7.46
butyronitrile	CCCC#N	ethanol		-5.62	-8.10	-9.15
piperidine	C1CCNCC1	ethanol		-6.22	-12.88	-12.31
benzylamine	NCc1ccccc1	ethanol		-8.14	-14.22	-14.94
2-methylpyridine	Cc1cccn1	ethanol		-6.27	-11.21	-10.56
3-methylpyridine	Cc1cccn1	ethanol		-6.28	-11.54	-10.51
3-chloropyridine	Clc1cccn1	ethanol		-7.24	-11.07	-11.78
difluoromethane	FCF	ethanol		-1.15	-2.76	-2.69
chlorodifluoromethane	FC(F)Cl	ethanol		-1.83	-3.78	-4.29
1,1,1,2-tetrafluoroethane	FCC(F)(F)F	ethanol		-2.13	-3.62	-3.78
1,1-difluoroethane	CC(F)F	ethanol		-2.14	-3.62	-4.18
naphthalene	c1ccc2ccccc2c1	ethanol		-7.32	-12.52	-12.57
tetramethylsilane	C[Si](C)(C)C	ethanol		-2.89	-5.31	-5.47
n-methylpyrrole	Cn1cccc1	ethanol		-5.17	-8.68	-9.63
difluoromethane	FCF	ethanol		-1.15	-4.31	-2.69
anthracene	c1ccc2cc3ccccc3cc2c1	ethanol		-10.54	-17.38	-17.51

water	O	ethanol		-4.14	-10.99	-10.27
tetramethylstannane	C[Sn](C)(C)C	ethanol		-3.75	-7.06	-6.79
propyl propanoate	CCCOC(=O)CC	pentane		-5.28	-9.22	-9.47
propyl butanoate	CCCOC(=O)CCC	pentane		-5.92	-10.01	-10.44
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	pentane		-5.54	-9.71	-9.16
undecane	CCCCCCCCCCC	hexane		-7.44	-13.44	-12.79
2,2-dimethylbutane	CCC(C)(C)C	hexane		-3.62	-6.64	-6.86
cyclopentane	C1CCCC1	hexane		-3.43	-6.76	-6.27
toluene	Cc1ccccc1	hexane		-4.76	-8.15	-8.54
bromobenzene	BrC1ccccc1	hexane		-5.67	-9.90	-9.96
1,2,4-trichlorobenzene	ClC1ccc(Cl)c(Cl)c1	hexane		-7.03	-12.41	-11.77
methanol	CO	hexane		-1.51	-3.61	-3.56
1-hexanol	CCCCCO	hexane		-5.13	-8.23	-9.35
2-methyl-1-pentanol	CCCC(C)CO	hexane		-4.95	-8.01	-9.12
1-nonanol	CCCCCCCCCO	hexane		-7.32	-13.78	-12.85
aniline	Nc1ccccc1	hexane		-5.70	-11.19	-9.91
pyridine	c1ccncc1	hexane		-4.79	-7.67	-8.35
2-chloropyridine	Clc1ccncc1	hexane		-5.90	-9.49	-10.12
butyronitrile	CCCC#N	hexane		-4.13	-7.57	-7.03
methyl ethyl ketone	CCC(C)=O	hexane		-3.58	-6.56	-6.71
tetrahydrofuran	C1CCOC1	hexane		-4.02	-6.89	-7.57
2-methyltetrahydrofuran	CC1CCCO1	hexane		-4.56	-7.56	-8.38
1,4-dioxane	C1COCCO1	hexane		-4.37	-7.45	-8.03
2,5,8-trioxanonane	COCCOCCOC	hexane		-5.54	-9.63	-9.80
2,5,8,11,14-pentaoxapentadecane	COCCOCCOCCOCCOC	hexane		-9.27	-16.16	-15.88
anisole	COc1ccccc1	hexane		-5.34	-9.74	-9.30
quinoline	c1ccc2ncccc2c1	hexane		-7.86	-12.00	-13.19
ethyl acetate	CCOC(C)=O	hexane		-3.82	-6.76	-7.19
pentyl acetate	CCCCOC(C)=O	hexane		-5.75	-10.16	-10.18
ethyl butanoate	CCCC(=O)OCC	hexane		-5.17	-8.77	-9.32
argon	[Ar]	hexane		0.43	-0.65	-0.37
krypton	[Kr]	hexane		-0.16	-1.13	-1.17
hydrogen	[H][H]	hexane		1.34	1.22	0.89
nitrogen	N#N	hexane		0.92	0.19	0.74
1-nitropropane	CCC[N+](=[O-])=O	hexane		-4.00	-7.81	-7.65
2-nitropropane	CC(C)[N+](=[O-])=O	hexane		-3.90	-7.46	-7.46
tetrachloromethane	ClC(Cl)(Cl)Cl	hexane		-4.19	-7.74	-7.42
methane	C	heptane		0.06	-0.91	-1.20
decane	CCCCCCCCCCC	heptane		-6.74	-12.28	-11.87
3-ethylpentane	CCC(CC)CC	heptane		-4.46	-8.41	-8.29
2,4-dimethylpentane	CC(C)CC(C)C	heptane		-4.37	-7.87	-8.13
tetralin	C1C=Cc2ccccc2C1	heptane		-6.92	-12.62	-11.83
pentanal	CCCC=O	heptane		-4.34	-7.45	-8.07
2-pentanone	CCCC(C)=O	heptane		-4.26	-7.74	-7.94
3-pentanone	CCC(=O)CC	heptane		-4.30	-7.89	-8.03
5-nonanone	CCCCC(=O)CCCC	heptane		-6.96	-11.97	-12.17
3-decanone	CCCCCCCC(=O)CC	heptane		-7.74		-13.34
6-undecanone	CCCCC(=O)CCCCC	heptane		-8.21	-14.18	-14.20
methyl propionate	CCC(=O)OC	heptane		-3.82	-7.05	-7.35
dimethyl malonate	COC(=O)CC(=O)OC	heptane		-5.48	-9.63	-10.05
n-butyl methyl ether	CCCCOC	heptane		-4.06	-7.36	-7.67
2,5,8,11-tetraoxododecane	CC(=O)CCC(=O)CCC(=O)CCC(C)=O	heptane		-9.75	-12.94	-16.20
1,3-dichloropropane	ClCCCCl	heptane		-4.49	-8.25	-8.17
2,2-dichloropropane	CC(C)(Cl)Cl	heptane		-4.31	-6.86	-7.88
1,2-dichlorobutane	CCC(Cl)CCl	heptane		-5.18	-8.75	-9.18
1-bromooctane	CCCCCCCCBr	heptane		-6.84	-12.81	-11.94
2-bromopropane	CC(C)Br	heptane		-3.62	-6.57	-7.03
1,2-dibromoethane	BrCCBr	heptane		-5.04	-8.68	-9.17
1,2-dibromopropane	CC(Br)CBr	heptane		-5.52	-9.13	-9.83
1,2-dibromobutane	CCC(Br)CBr	heptane		-6.09	-10.18	-10.67
1,11-dibromoundecane	BrCCCCCCCCCCCBr	heptane		-9.77		-15.99
2-iodobutane	CCC(C)I	heptane		-5.10	-8.56	-8.72
methanol	CO	heptane		-1.48	-3.56	-3.71
1-propanol	CCCO	heptane		-2.94	-5.28	-6.08
isopropanol	CC(C)O	heptane		-2.79	-5.40	-5.87
2-methyl-2-butanol	CCC(C)(C)O	heptane		-4.01	-6.32	-8.03
1-hexanol	CCCCCO	heptane		-5.12	-9.16	-9.53
2-methoxyethanol	COCCO	heptane		-3.75	-8.18	-7.81
isopropylamine	CC(C)N	heptane		-2.67	-5.47	-5.67
iso-butylamine	CC(C)CN	heptane		-3.44	-6.72	-6.94
undecylamine	CCCCCCCCCCCN	heptane		-8.67		-15.48
hexadecylamine	CCCCCCCCCCCCCCCCN	heptane		-12.31		-21.31
dibutylamine	CCCNCCCC	heptane		-6.20	-11.46	-11.80
tripropylamine	CCCN(CCC)CCC	heptane		-6.59	-10.96	-12.18
piperidine	C1CCNCC1	heptane		-5.14	-8.17	-9.60
heptamethylenimine	C1CCCCCCC1	heptane		-6.28	-10.13	-11.57
toluene	Cc1ccccc1	heptane		-4.79	-8.59	-8.80
butyronitrile	CCCC#N	heptane		-3.97	-6.83	-6.84
heptanonitrile	CCCCCCC#N	heptane		-6.18	-10.18	-10.40
tetradecanenitrile	CCCCCCCCCCCCC#N	heptane		-10.62	-18.59	-17.32
hydrogen	[H][H]	heptane		1.41	0.90	0.95

nitromethane	C[N+](=O)[O-]	heptane	-2.24	-5.83	-4.80
1-butanethiol	CCCCS	heptane	-4.76	-8.08	-8.11
ethyl benzoate	CCOC(=O)c1ccccc1	heptane	-7.20	-12.69	-12.51
3-methylpyridine	Cc1ccncc1	heptane	-5.36	-9.03	-9.36
4-methylpyridine	Cc1ccncc1	heptane	-5.35	-8.92	-9.32
1-propanol	CCCO	octane	-2.92	-5.98	-6.22
1-butanol	CCCCO	octane	-3.65	-7.15	-7.42
1-nonanol	CCCCCCCCCO	octane	-7.28	-13.32	-13.15
1-undecanol	CCCCCCCCCCCCO	octane	-8.50	-15.39	-15.13
hydrogen	[H][H]	octane	1.45	0.97	0.97
carbon dioxide	O=C=O	octane	0.10	-1.94	-1.28
methyl hexanoate	CCCCCC(=O)OC	octane	-5.81	-10.47	-10.58
methyl heptanoate	CCCCCCC(=O)OC	octane	-6.39	-11.84	-11.50
methyl nonanoate	CCCCCCCC(=O)OC	octane	-7.67	-13.97	-13.49
ethyl acetate	CCOC(C)=O	octane	-3.70	-6.96	-7.27
1-chlorobutane	CCCCl	octane	-3.93	-7.51	-7.60
water	O	octane	-0.97	-2.49	-3.30
helium	[He]	nonane	1.83	2.32	1.68
krypton	[Kr]	nonane	0.08	-1.11	-1.19
methane	C	decane	0.19	-1.03	-1.06
isobutane	CC(C)C	decane	-2.08	-3.98	-4.89
2,2-dimethylbutane	CCC(C)(C)C	decane	-3.24	-6.56	-6.75
1-hexene	CCCC=C	decane	-3.71	-7.23	-7.47
methyl hexanoate	CCCCCC(=O)OC	decane	-5.69	-10.44	-10.54
methyl heptanoate	CCCCCCC(=O)OC	decane	-6.26	-11.65	-11.47
1-chloronaphthalene	Clc1cccc2cccc12	decane	-8.01	-14.80	-14.05
sulfur hexafluoride	F[S](F)(F)(F)(F)F	decane	-0.09	-1.89	-1.64
pyridine	c1ccncc1	decane	-4.34	-7.51	-7.99
2-pentanone	CCCC(C)=O	decane	-4.15	-7.67	-8.12
water	O	decane	-1.01	-1.65	-3.53
undecane	CCCCCCCCCCCC	undecane	-7.40	-13.46	-13.44
1-hexanol	CCCCCCO	undecane	-4.97	-9.06	-9.73
dodecane	CCCCCCCCCCCCC	dodecane	-8.04	-14.75	-14.47
diethyl ether	CCOCC	dodecane	-2.92	-6.08	-6.22
dipropyl ether	CCCOCC	dodecane	-4.39	-8.24	-8.55
krypton	[Kr]	dodecane	0.21	-1.02	-1.16
xenon	[Xe]	dodecane	-0.65	-2.28	-2.56
carbon dioxide	O=C=O	dodecane	0.29	-1.43	-1.21
1-propanol	CCCO	dodecane	-2.57	-5.41	-5.95
water	O	dodecane	-1.03	-2.25	-3.64
dipropyl ether	CCCOCC	tetradecane	-4.29	-8.05	-8.31
2-octanone	CCCCCCC(=O)C	tetradecane	-5.90	-11.06	-10.75
15-crown-5	C1COCCOCCOCCOCCO1	tetradecane	-8.85	-18.11	-16.66
heptane	CCCCCCC	hexadecane	-4.29	-8.64	-8.48
cyclopentane	C1CCCC1	hexadecane	-3.38	-6.61	-7.09
2-heptanone	CCCCCCC(=O)C	hexadecane	-5.22	-9.67	-9.83
diethyl ether	CCOCC	hexadecane	-2.87	-6.02	-6.21
dipropyl ether	CCCOCC	hexadecane	-4.33	-8.16	-8.50
dichloromethane	ClCCl	hexadecane	-2.77	-5.54	-5.83
ethanol	CCO	hexadecane	-1.83	-3.90	-4.82
heptan-1-ol	CCCCCCCCO	hexadecane	-5.53	-10.62	-10.85
1-nonanol	CCCCCCCCCO	hexadecane	-7.11	-12.62	-13.32
anisole	COc1ccccc1	hexadecane	-5.06	-9.86	-9.51
fluorobenzene	Fc1ccccc1	hexadecane	-3.58	-7.42	-7.26
heptylamine	CCCCCCCCN	hexadecane	-5.37	-10.82	-10.72
decylamine	CCCCCCCCCCN	hexadecane	-7.48	-14.35	-14.37
tert-butylamine	CC(C)(C)N	hexadecane	-2.82	-6.25	-6.92
helium	[He]	hexadecane	1.64	1.97	1.48
diiodomethane	ICI	hexadecane	-5.45	-9.31	-9.24
diisopropyl ether	CC(C)OC(C)C	hexadecane	-3.96	-7.33	-7.88
3-ethylpentane	CCC(CC)CC	1-octanol	-3.77	-8.18	-7.93
decane	CCCCCCCCC	1-octanol	-6.23	-11.88	-11.93
hexadecane	CCCCCCCCCCCCCCCC	1-octanol	-10.31	-18.69	-18.62
tetrafluoromethane	FC(F)(F)F	1-octanol	0.83	0.22	-0.75
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	1-octanol	-4.70	-6.32	-8.69
1-chloropropane	CCCCl	1-octanol	-2.96	-6.22	-6.19
1-chlorohexane	CCCCCCC	1-octanol	-5.00	-9.66	-9.46
methyl acetate	COC(C)=O	1-octanol	-2.84	-5.88	-5.39
tert-butanol	CC(C)(C)O	1-octanol	-4.25	-11.23	-9.87
pentan-1-ol	CCCCCO	1-octanol	-6.13	-13.56	-13.12
benzene	c1ccccc1	1-octanol	-3.73	-7.40	-7.22
1,2,3-trichlorobenzene	Clc1cccc(Cl)c1Cl	1-octanol	-7.25	-13.31	-12.87
hexachlorobenzene	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	1-octanol	-9.36	-17.97	-16.61
diethylamine	CCNCC	1-octanol	-4.53	-10.16	-10.55
argon	[Ar]	1-octanol	1.10	-0.16	0.23
oxygen	O=O	1-octanol	0.76	-0.28	-0.61
3-chlorobiphenyl	Clc1cccc(c1)c2ccccc2	1-octanol	-9.82	-15.88	-16.31
2,3,3',4,4'-pentachlorobiphenyl	Clc1ccc(cc1Cl)c2ccc(Cl)c(Cl)c2Cl	1-octanol	-13.13	-21.41	-21.10
2,2',4,4',5,5'-hexachlorobiphenyl	Clc1cc(Cl)c(cc1Cl)c2cc(Cl)c(Cl)c2Cl	1-octanol	-13.60	-20.98	-21.32
1,3,5-trichloronaphthalene	Clc1cc(Cl)c2ccccc(Cl)c2c1	1-octanol	-10.52	-17.33	-17.25
1,4,5,8-tetrachloronaphthalene	Clc1ccc(Cl)c2c(Cl)ccc(Cl)c12	1-octanol	-11.57	-19.25	-19.38
tetradecane	CCCCCCCCCCCCCCC	acetonitrile	-8.01	-11.78	-14.20

2-methylpentane	CCCC(C)C	acetonitrile	-2.57	-4.77	-5.27
1-propanol	CCCO	acetonitrile	-4.86	-8.95	-10.45
1-pentanol	CCCCCO	acetonitrile	-5.84	-10.90	-12.07
2-butanol	CCC(C)O	acetonitrile	-5.15	-9.59	-10.95
benzene	c1ccccc1	acetonitrile	-4.18	-7.49	-7.63
ethylbenzene	CCc1ccccc1	acetonitrile	-5.30	-9.92	-9.33
m-xylene	Cc1cccc(C)c1	acetonitrile	-5.21	-10.03	-9.23
nitroethane	CC[N+](=O)[O-]	acetonitrile	-5.20	-9.46	-9.33
propionitrile	CCC#N	acetonitrile	-5.10	-8.58	-8.10
dichloromethane	ClCCl	acetonitrile	-3.34	-7.50	-6.42
acetone	CC(C)=O	acetonitrile	-3.56	-7.86	-6.46
methyl ethyl ketone	CCC(C)=O	acetonitrile	-4.18	-8.32	-7.39
ethylenediamine	NCCN	acetonitrile	-6.56	-9.32	-13.78
heptyl methyl ether	CCCCCCCOC	acetonitrile	-5.54	-9.71	-9.94
ethyl hexyl ether	CCCCCCCCOC	acetonitrile	-5.42		-9.74
butyl isobutyl ether	CCCCOCC(C)C	acetonitrile	-5.33		-9.67
nitric oxide	[N]=O	acetonitrile	0.55	-0.44	-0.50
methyl isobutyrate	COC(=O)C(C)C	acetonitrile	-4.55	-8.63	-7.99
methyl benzoate	COC(=O)c1ccccc1	acetonitrile	-7.36	-12.81	-12.07
pyridine	c1ccncc1	acetonitrile	-5.72	-8.60	-9.40
4-chlorophenol	Oc1ccc(Cl)cc1	acetonitrile	-8.94	-16.09	-16.24
4-bromophenol	Oc1ccc(Br)cc1	acetonitrile	-9.64	-18.16	-17.59
2-methoxyphenol	COc1ccccc1O	acetonitrile	-9.09	-14.84	-17.20
4-methoxyphenol	COc1ccc(O)cc1	acetonitrile	-9.65	-18.76	-17.64
naphthalene	c1ccc2ccccc2c1	acetonitrile	-7.07	-12.12	-11.99
imidazole	[nH]1ccnc1	acetonitrile	-8.85	-15.07	-15.88
1,4-dibromobenzene	BrC1=CC(=CC=C1)Br	acetonitrile	-7.25	-11.89	-12.10
1,4-diiodobenzene	Ic1ccc(I)cc1	acetonitrile	-9.10	-14.03	-14.22
2-bromotoluene	Cc1ccccc1Br	acetonitrile	-5.96	-11.42	-9.99
4-iodotoluene	Cc1ccc(I)cc1	acetonitrile	-6.93	-11.13	-11.21
2,4-dinitrotoluene	Cc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-]	acetonitrile	-11.01	-18.64	-18.65
acetamide	CC(N)=O	acetonitrile	-7.64	-14.05	-15.04
4-nitrophenol	Oc1ccc(cc1)[N+](=O)[O-]	acetonitrile	-10.97	-19.91	-19.93
1,3-dihydroxybenzene	Oc1ccccc1O	acetonitrile	-10.68	-20.51	-20.60
1,4-dihydroxybenzene	Oc1ccc(O)cc1	acetonitrile	-10.93	-20.43	-21.08
2,4-di-tert-butylphenol	CC(C)(C)c1ccc(O)c(c1)C(C)(C)C	acetonitrile	-10.99	-18.95	-20.55
2-adamantanone	O=C1C2CC3CC(C2)CC1C3	acetonitrile	-9.50	-16.71	-15.39
1,3-dicyanobenzene	N#Cc1cccc(c1)C#N	acetonitrile	-10.68	-16.49	-15.46
1-cyanonaphthalene	N#Cc1cccc2ccccc12	acetonitrile	-11.29	-16.06	-17.55
9-cyanoanthracene	N#Cc1c2ccccc2cc3ccccc13	acetonitrile	-14.37		-22.32
methane	C	acetone	0.10	-0.67	-0.85
hexane	CCCCCC	acetone	-3.22	-5.77	-6.01
1-propanol	CCCO	acetone	-5.12	-10.24	-10.50
isobutanol	CC(C)CO	acetone	-5.66	-10.57	-11.34
2-methyl-2-butanol	CCC(C)(C)O	acetone	-4.87	-10.36	-9.77
helium	[He]	acetone	2.09	2.75	2.16
neon	[Ne]	acetone	1.92	2.41	1.83
hydrogen	[H][H]	acetone	1.44	1.08	0.98
carbon monoxide	C=O	acetone	0.45	0.06	-0.29
iodomethane	CI	acetone	-3.16	-6.37	-5.45
1-iodobutane	CCCCI	acetone	-4.82	-8.79	-7.96
2-iodo-2-methylpropane	CC(C)(C)I	acetone	-4.52	-7.66	-7.55
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	acetone	-6.91	-12.73	-11.75
cis-1,2-dichloroethene	Cl/C=C/Cl	acetone	-3.86	-8.31	-7.01
chloroform	ClC(Cl)Cl	acetone	-4.44	-8.28	-7.98
acetone	CC(C)=O	acetone	-3.83	-7.62	-6.93
methyl ethyl ketone	CCC(C)=O	acetone	-4.37	-8.20	-7.67
carbon disulfide	S=C=S	acetone	-3.01	-5.78	-3.74
methyl tert-butyl ether	COC(C)(C)C	acetone	-3.45	-6.70	-6.16
tetrahydrofuran	C1CCOC1	acetone	-3.60	-7.72	-6.06
1,3,5-trioxane	C1OCOC1	acetone	-4.81	-9.97	-8.08
18-crown-6	C1COCCOCCOCCOCCOCCO1	acetone	-11.53	-22.39	-21.39
triethylamine	CCN(CC)CC	acetone	-4.28	-7.24	-8.33
1-adamantanol	OC12CC3CC(CC(C3)C1)C2	acetone	-9.49	-15.25	-16.12
tetramethylstannane	C[Sn](C)(C)C	acetone	-3.67	-6.05	-5.90
methylformamide	CNC=O	acetone	-6.98	-12.17	-13.37
n-methylbutyrolactam	CN1CCCC1=O	acetone	-7.14	-13.77	-12.35
ethane	CC	cyclohexane	-0.82	-2.66	-2.21
nonane	CCCCCCCCC	cyclohexane	-6.00	-10.63	-10.35
hexadecane	CCCCCCCCCCCCCCCC	cyclohexane	-10.93	-18.48	-18.14
2,2-dimethylpropane	CC(C)(C)C	cyclohexane	-2.88	-5.80	-5.56
2-methyloctane	CCCCCCC(C)C	cyclohexane	-5.89	-10.30	-10.21
cyclooctane	C1CCCCCCC1	cyclohexane	-5.58	-10.39	-9.48
1-dodecene	CCCCCCCCCCC=C	cyclohexane	-8.15	-13.92	-13.82
1,5-hexadiene	C=CCCC=C	cyclohexane	-3.96	-7.02	-7.16
4-octyne	CCCC#CCCC	cyclohexane	-5.36	-9.68	-9.35
1-chlorooctane	CCCCCCCCCl	cyclohexane	-6.82	-12.30	-11.59
chlorotrifluoromethane	FC(F)(F)Cl	cyclohexane	-0.45	-2.22	-2.18
1-iodobutane	CCCCI	cyclohexane	-5.32	-8.50	-8.80
3-pentanone	CCC(=O)CC	cyclohexane	-4.52	-7.27	-8.08
2-hexanone	CCCCC(C)=O	cyclohexane	-5.19	-8.64	-9.13
3-hexanone	CCCC(=O)CC	cyclohexane	-5.24	-8.25	-9.25

dipropyl ether	CCCOCCC	cyclohexane	-4.72	-8.15	-8.33
tetrahydropyran	C1CCOCC1	cyclohexane	-4.76	-8.03	-8.49
12-crown-4	C1COCCOCCOCCO1	cyclohexane	-8.23	-13.10	-14.95
18-crown-6	C1COCCOCCOCCOCCOCCO1	cyclohexane	-12.22	-20.02	-22.36
1-propanol	CCCO	cyclohexane	-3.15	-5.38	-6.13
1-butanol	CCCCO	cyclohexane	-3.88	-6.62	-7.33
1-pentanol	CCCCCO	cyclohexane	-4.55	-7.60	-8.39
1-undecanol	CCCCCCCCCCCCO	cyclohexane	-8.71	-14.68	-15.02
2-methyl-2-butanol	CCC(C)(C)O	cyclohexane	-4.19	-6.08	-8.04
butyl acetate	CCCCOC(C)=O	cyclohexane	-5.32	-8.94	-9.42
ethyl benzoate	CCOC(=O)c1ccccc1	cyclohexane	-7.60	-12.48	-12.91
butyronitrile	CCCC#N	cyclohexane	-4.31	-6.93	-7.06
toluene	Cc1ccccc1	cyclohexane	-4.89	-8.38	-8.64
1,2,4-trimethylbenzene	Cc1ccc(C)c(C)c1	cyclohexane	-6.17	-10.57	-10.59
phenanthrene	c1ccc2c(c1)ccc3ccccc23	cyclohexane	-10.35	-16.42	-17.27
acetophenone	CC(=O)c1ccccc1	cyclohexane	-6.69	-10.20	-11.39
bromobenzene	BrC1ccccc1	cyclohexane	-5.75	-9.40	-9.92
chlorobenzene	ClC1ccccc1	cyclohexane	-5.29	-8.89	-9.16
n-methylaniline	CNc1ccccc1	cyclohexane	-6.33	-10.42	-11.04
3-methylphenol	Cc1cccc(O)c1	cyclohexane	-5.97	-8.73	-10.33
argon	[Ar]	cyclohexane	0.50	-0.22	-0.22
nitrogen	N#N	cyclohexane	0.91	0.51	0.84
nitric oxide	[N]=O	cyclohexane	0.32	-1.07	-0.43
2-methylpyridine	Cc1ccccn1	cyclohexane	-5.49	-8.59	-9.25
3-methylpyridine	Cc1cccn1	cyclohexane	-5.49	-8.63	-9.22
2,4-dimethylpyridine	Cc1ccnc(C)c1	cyclohexane	-6.21	-9.53	-10.42
3-chloropyridine	Clc1cccn1	cyclohexane	-6.17	-9.97	-10.34
dimethyl sulfoxide	C[S](C)=O	cyclohexane	-6.32	-8.46	-11.55
n-pentylamine	CCCCCN	cyclohexane	-4.55	-8.11	-8.49
n-hexylamine	CCCCCCN	cyclohexane	-5.00	-9.46	-9.26
decylamine	CCCCCCCCCN	cyclohexane	-7.91	-13.90	-14.12
ethyl benzoate	CCOC(=O)c1ccccc1	cyclohexane	-7.60	-12.56	-12.91
benzil	O=C(c1ccccc1)C(=O)c2ccccc2	cyclohexane	-11.48	-15.77	-18.69
2-iodo-2-methylpropane	CC(C)(C)I	cyclohexane	-4.86	-7.98	-7.98
1-bromoadamantane	BrC12CC3CC(C(C3)C1)C2	cyclohexane	-8.82	-13.96	-14.22
1-chloro-4-nitrobenzene	[O-][N+](=O)c1ccc(Cl)cc1	cyclohexane	-7.26	-11.45	-12.56
hexane	CCCCCC	benzene	-3.84	-6.37	-6.64
nonane	CCCCCCCCC	benzene	-5.96	-9.48	-9.98
pentadecane	CCCCCCCCCCCCCCC	benzene	-10.16	-16.11	-16.65
heptadecane	CCCCCCCCCCCCCCCCC	benzene	-11.50	-18.08	-18.93
2,2,5,5-tetramethylhexane	CC(C)(C)CCC(C)(C)C	benzene	-6.00	-8.23	-10.31
cyclopentane	C1CCCC1	benzene	-3.51	-6.13	-5.94
cis-decalin	C1CC[C@@H]2CCCC[C@H]2C1	benzene	-6.87	-11.10	-10.71
1-decene	CCCCCCCC=C	benzene	-6.70	-10.89	-11.14
1-tridecene	CCCCCCCCCCCCC=C	benzene	-8.86	-14.12	-14.62
trans-4-octene	CCC/C=C/CCC	benzene	-5.35	-8.44	-9.00
1,3-butadiene	C=CC=C	benzene	-2.64	-4.85	-4.82
1-methylcyclohexene	CC1=CCCCC1	benzene	-5.05	-8.35	-8.52
methyl ethyl ketone	CCC(C)=O	benzene	-4.41	-8.19	-7.95
3-hexanone	CCCC(=O)CC	benzene	-5.72	-10.03	-9.98
2-decanone	CCCCCCCCC(C)=O	benzene	-8.25	-14.01	-13.77
2-undecanone	CCCCCCCCC(C)=O	benzene	-8.91	-15.01	-14.76
cyclohexanone	O=C1CCCCC1	benzene	-6.20	-11.03	-10.68
dimethyl ether	COC	benzene	-2.65	-5.04	-5.07
diethyl ether	CCOCC	benzene	-3.94	-6.30	-7.12
dibutyl ether	CCCCOCCCC	benzene	-6.35	-10.08	-10.74
1,3-dioxane	C1COCOC1	benzene	-5.06	-9.51	-9.05
2-methyltetrahydrofuran	CC1CCCO1	benzene	-5.12	-8.16	-9.04
ethanol	CCO	benzene	-2.84	-7.08	-5.60
chloroethane	CCCl	benzene	-2.83	-6.12	-5.17
2-chloro-2-methylpropane	CC(C)(C)Cl	benzene	-4.12	-6.72	-7.34
4-methylpyridine	Cc1ccncc1	benzene	-6.12	-10.76	-10.21
3-bromopyridine	BrC1cccn1	benzene	-7.28	-11.87	-12.11
tert-butylamine	CC(C)(C)N	benzene	-3.54	-6.98	-7.05
tripropylamine	CCCN(CCC)CCC	benzene	-6.67	-9.92	-11.87
nitrogen	N#N	benzene	0.86	1.02	0.94
sulfur dioxide	O=[S]=O	benzene	-2.89	-5.80	-5.81
methyl benzoate	COC(=O)c1ccccc1	benzene	-7.76	-13.24	-13.25
butyl benzoate	CCCCOC(=O)c1ccccc1	benzene	-9.53	-16.32	-15.90
1,4-dibromobenzene	BrC1ccc(Br)cc1	benzene	-7.65	-13.04	-12.77
4-iodotoluene	Cc1ccc(I)cc1	benzene	-7.83	-12.27	-12.63
1-nitronaphthalene	[O-][N+](=O)c1cccc2ccccc12	benzene	-10.06	-16.30	-17.06
4-chloro-1-nitrobenzene	[O-][N+](=O)c1ccc(Cl)cc1	benzene	-8.02	-13.20	-13.85
4-bromoaniline	Nc1ccc(Br)cc1	benzene	-8.67	-14.29	-14.87
1-chloro-3-nitrobenzene	[O-][N+](=O)c1cccc(Cl)c1	benzene	-7.96	-13.84	-13.73
4-iodoaniline	Nc1ccc(I)cc1	benzene	-9.81	-15.20	-16.32
3-nitroaniline	Nc1cccc(c1)[N+](=O)[O-]	benzene	-9.61	-16.85	-17.26
2-methoxyphenol	COc1ccccc1O	benzene	-7.64	-13.36	-13.71
4-hydroxy-3-methoxybenzaldehyde	COc1cc(C=O)ccc1O	benzene	-9.22	-17.38	-16.08
2,4-dichlorophenol	Oc1ccc(Cl)cc1Cl	benzene	-8.35	-13.03	-14.09
2,4,6-trinitrophenol	Oc1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	benzene	-10.37	-21.32	-18.22

	<chem>[O-][N+](O-)[O-][N+](O-)=O</chem>					
5-methyl-1,10-phenanthroline	<chem>Cc1cc2ccnc2c3ncccc13</chem>	benzene		-13.51	-21.69	-22.10
heptane	<chem>CCCCCCC</chem>	dimethyl sulfoxide		-2.41	-5.05	-6.07
1,3-butadiene	<chem>C=CC=C</chem>	dimethyl sulfoxide		-1.73	-4.06	-5.16
4-octyne	<chem>CCCC#CCCC</chem>	dimethyl sulfoxide		-4.13	-8.49	-8.86
toluene	<chem>Cc1ccccc1</chem>	dimethyl sulfoxide		-3.88	-8.22	-8.23
ethylbenzene	<chem>CCc1ccccc1</chem>	dimethyl sulfoxide		-4.50	-8.92	-9.16
propylbenzene	<chem>CCc1ccccc1</chem>	dimethyl sulfoxide		-5.06	-9.53	-10.05
isopropylbenzene	<chem>CC(C)c1ccccc1</chem>	dimethyl sulfoxide		-5.03	-9.48	-10.06
heptylbenzene	<chem>CCCCCCCc1ccccc1</chem>	dimethyl sulfoxide		-7.54	-12.47	-14.11
n-heptylamine	<chem>CCCCCCN</chem>	dimethyl sulfoxide		-5.17	-10.31	-12.70
acetone	<chem>CC(C)=O</chem>	dimethyl sulfoxide		-2.91	-7.14	-6.76
2-pentanone	<chem>CCCC(C)=O</chem>	dimethyl sulfoxide		-4.03	-8.48	-8.47
2-heptanone	<chem>CCCCC(C)=O</chem>	dimethyl sulfoxide		-4.92	-9.80	-9.82
2-octanone	<chem>CCCCC(C)=O</chem>	dimethyl sulfoxide		-5.43	-10.49	-10.58
diisopropyl ether	<chem>CC(C)OC(C)C</chem>	dimethyl sulfoxide		-3.23	-6.34	-7.40
methyl <i>tert</i> -butyl ether	<chem>COC(C)(C)C</chem>	dimethyl sulfoxide		-2.52	-5.79	-6.22
ethyl <i>tert</i> -butyl ether	<chem>CCOC(C)(C)C</chem>	dimethyl sulfoxide		-3.06	-6.57	-7.17
1,2-diethoxyethane	<chem>CCOCCOCC</chem>	dimethyl sulfoxide		-5.08	-9.36	-10.33
furan	<chem>c1ccccc1</chem>	dimethyl sulfoxide		-2.95	-7.17	-6.60
15-crown-5	<chem>C1COCCOCCOCCOCCO1</chem>	dimethyl sulfoxide		-10.32	-18.85	-21.56
1-chlorooctane	<chem>CCCCCCCCCl</chem>	dimethyl sulfoxide		-5.69	-9.51	-11.46
dibromomethane	<chem>BrCBr</chem>	dimethyl sulfoxide		-3.66	-9.37	-8.28
1-pentanenitrile	<chem>CCCC#N</chem>	dimethyl sulfoxide		-5.46	-9.81	-10.00
1-octanenitrile	<chem>CCCCCCC#N</chem>	dimethyl sulfoxide		-7.09	-11.92	-12.81
1-undecanenitrile	<chem>CCCCCCCCC#N</chem>	dimethyl sulfoxide		-8.29	-14.26	-14.51
1-tridecanenitrile	<chem>CCCCCCCCC#N</chem>	dimethyl sulfoxide		-9.62	-15.81	-17.25
ethanol	<chem>CCO</chem>	dimethyl sulfoxide		-3.63	-9.83	-9.77
1-propanol	<chem>CCCO</chem>	dimethyl sulfoxide		-4.18	-10.46	-10.66
1-heptanol	<chem>CCCCCCO</chem>	dimethyl sulfoxide		-6.26	-13.93	-13.96
1-undecanol	<chem>CCCCCCCCCO</chem>	dimethyl sulfoxide		-8.49	-16.93	-17.56
cyclohexanol	<chem>OC1CCCCC1</chem>	dimethyl sulfoxide		-6.35	-12.94	-14.01
methyl acetate	<chem>COC(C)=O</chem>	dimethyl sulfoxide		-3.41	-7.26	-7.27
ethyl acetate	<chem>CCOC(C)=O</chem>	dimethyl sulfoxide		-3.72	-7.84	-7.83
nitromethane	<chem>C[N+](O-)=O</chem>	dimethyl sulfoxide		-4.24	-9.31	-9.28
<i>n</i> -methylpyrrole	<chem>Cn1ccccc1</chem>	dimethyl sulfoxide		-4.25	-9.60	-9.25
acetaldehyde	<chem>CC=O</chem>	dimethyl sulfoxide		-2.20	-6.41	-5.63
vinyl acetate	<chem>CC(=O)OC=C</chem>	dimethyl sulfoxide		-4.05	-7.26	-8.30
1-adamantanol	<chem>OC12CC3CC(CC(C3)C1)C2</chem>	dimethyl sulfoxide		-9.63	-15.77	-18.96
heptane	<chem>CCCCCCC</chem>	propylene carbonate		-2.63	-5.89	-6.16
decane	<chem>CCCCCCCCC</chem>	propylene carbonate		-4.26	-9.08	-8.74
1-hexene	<chem>CCCC=C</chem>	propylene carbonate		-2.73	-5.93	-6.44
isobutyl acetate	<chem>CC(C)COC(C)=O</chem>	propylene carbonate		-4.77	-8.64	-9.80
butyl propanoate	<chem>CCCCOC(=O)CC</chem>	propylene carbonate		-5.11	-11.22	-10.26
benzyl alcohol	<chem>OCc1ccccc1</chem>	propylene carbonate		-7.69	-13.72	-15.46
2-phenylethanol	<chem>OCCc1ccccc1</chem>	propylene carbonate		-7.71	-14.91	-15.19
3-phenyl-1-propanol	<chem>OCCCc1ccccc1</chem>	propylene carbonate		-8.15	-15.54	-15.88
methyl <i>tert</i> -butyl ether	<chem>COC(C)(C)C</chem>	propylene carbonate		-2.79	-6.95	-6.43
1,4-dioxane	<chem>C1COCCO1</chem>	propylene carbonate		-4.20	-9.32	-8.34
ethanol	<chem>CCO</chem>	propylene carbonate		-3.09	-8.09	-8.25
propan-2-ol	<chem>CC(C)O</chem>	propylene carbonate		-3.32	-8.32	-8.54
<i>tert</i> -butanol	<chem>CC(C)(C)O</chem>	propylene carbonate		-2.98	-8.63	-7.91
2-methyl-1-butanol	<chem>CCC(C)CO</chem>	propylene carbonate		-4.26	-9.54	-10.18
3-methyl-2-butanol	<chem>CC(C)(C)CO</chem>	propylene carbonate		-3.68	-9.28	-9.22
2-chloro-2-methylpropane	<chem>CC(C)(C)Cl</chem>	propylene carbonate		-2.99	-6.21	-6.85
2-bromo-2-methylpropane	<chem>CC(C)(C)Br</chem>	propylene carbonate		-3.34	-6.77	-7.65
decane	<chem>CCCCCCCCC</chem>	carbon tetrachloride		-6.70	-11.56	-11.74
2-methylbutane	<chem>CCC(C)C</chem>	carbon tetrachloride		-2.98	-5.72	-5.86
cyclopentane	<chem>C1CCCC1</chem>	carbon tetrachloride		-3.55	-6.80	-6.63
adamantane	<chem>C1C2CC3CC1CC(C2)C3</chem>	carbon tetrachloride		-7.29	-11.57	-11.58
ethene	<chem>C=C</chem>	carbon tetrachloride		-0.73	-2.29	-2.28
1-heptene	<chem>CCCCCC=C</chem>	carbon tetrachloride		-4.55	-8.42	-8.32
2-heptanone	<chem>CCCCC(C)=O</chem>	carbon tetrachloride		-6.06	-11.09	-10.79
5-nonanone	<chem>CCCCC(=O)CCCC</chem>	carbon tetrachloride		-7.42	-13.09	-12.98
cyclopentanone	<chem>O=C1CCCC1</chem>	carbon tetrachloride		-4.99	-9.89	-8.90
cyclohexanone	<chem>O=C1CCCCC1</chem>	carbon tetrachloride		-5.72	-10.68	-10.05
diethyl ether	<chem>CCOCC</chem>	carbon tetrachloride		-3.56	-6.92	-6.86
dibutyl ether	<chem>CCCCOCCCC</chem>	carbon tetrachloride		-6.20	-11.10	-10.98
1,2-dimethoxyethane	<chem>COCCOC</chem>	carbon tetrachloride		-4.23	-8.96	-7.80
1,2-diethoxyethane	<chem>CCOCCOCC</chem>	carbon tetrachloride		-5.37	-10.87	-9.58
12-crown-4	<chem>C1COCCOCCOCCO1</chem>	carbon tetrachloride		-8.47	-15.27	-15.73
chloroform	<chem>ClC(Cl)Cl</chem>	carbon tetrachloride		-3.71	-7.20	-6.81
<i>cis</i> -1,2-dichloroethylene	<chem>Cl/C=C/Cl</chem>	carbon tetrachloride		-3.30	-6.60	-6.28
iodomethane	<chem>CI</chem>	carbon tetrachloride		-3.42	-6.48	-6.24
1-nitropropane	<chem>CCC[N+](O-)=O</chem>	carbon tetrachloride		-4.62	-9.14	-8.71
butyl acetate	<chem>CCCCOC(C)=O</chem>	carbon tetrachloride		-5.55	-10.57	-10.10
ethylbenzene	<chem>CCc1ccccc1</chem>	carbon tetrachloride		-5.61	-10.00	-9.97
anisole	<chem>COc1ccccc1</chem>	carbon tetrachloride		-5.78	-10.82	-10.21
1,2-dibromobenzene	<chem>BrC1ccccc1Br</chem>	carbon tetrachloride		-7.46	-12.47	-12.93
1,3,5-tribromobenzene	<chem>BrC1C(Br)C(Br)C1</chem>	carbon tetrachloride		-8.89	-14.50	-15.00
chlorobenzene	<chem>Clc1ccccc1</chem>	carbon tetrachloride		-5.35	-9.64	-9.50
1,2-dichlorobenzene	<chem>Clc1ccccc1Cl</chem>	carbon tetrachloride		-6.35	-11.03	-11.03
hexachlorobenzene	<chem>Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl</chem>	carbon tetrachloride		-9.70	-17.08	-16.37



iodobenzene	Ic1ccccc1	carbon tetrachloride		-6.68	-11.47	-11.12
1,3-diiodobenzene	Ic1ccccc1Ic1	carbon tetrachloride		-9.07	-15.07	-14.20
1,4-diiodobenzene	Ic1ccccc1Icc1	carbon tetrachloride		-9.07	-15.09	-14.18
3-iodotoluene	Cc1ccccc1Ic1	carbon tetrachloride		-7.40	-12.22	-12.22
nitrobenzene	[O-][N+](=O)c1ccccc1	carbon tetrachloride		-6.34	-12.00	-11.20
2,4-dimethylpyridine	Cc1ccnc(C)c1	carbon tetrachloride		-6.47	-11.68	-11.14
3-chloropyridine	C1c1ccnc1	carbon tetrachloride		-6.25	-11.62	-10.59
triethylamine	CCN(CC)CC	carbon tetrachloride		-4.72	-9.09	-9.11
hydrogen	[H][H]	carbon tetrachloride		1.51	1.38	1.08
carbon tetrafluoride	FC(F)(F)F	carbon tetrachloride		0.91	0.14	-0.13
dimethyl sulfide	CSC	carbon tetrachloride		-3.21	-5.59	-5.84
4-bromophenol	Oc1ccc(Br)cc1	carbon tetrachloride		-7.56	-14.27	-13.37
diethyl carbonate	CCOC(=O)OCC	carbon tetrachloride		-5.24	-10.23	-9.73
ethane	CC	toluene		-0.78	-2.13	-1.99
cyclohexane	C1CCCCC1	toluene		-4.15	-7.30	-7.09
acetone	CC(C)=O	toluene		-3.49	-7.19	-6.48
4-heptanone	CCCC(=O)CCC	toluene		-6.12	-11.19	-10.54
cyclohexanone	O=C1CCCCC1	toluene		-6.01	-11.03	-10.35
butyl methyl ether	CCCCOC	toluene		-4.22	-7.78	-7.48
chloroform	ClC(Cl)Cl	toluene		-4.08	-8.08	-7.16
butylamine	CCCCN	toluene		-4.05	-8.04	-7.61
triethylamine	CCN(CC)CC	toluene		-4.59	-8.27	-8.49
helium	[He]	toluene		1.97	2.42	1.98
argon	[Ar]	toluene		0.59	0.23	-0.07
chlorine	[Cl][Cl]	toluene		-1.53	-5.73	-3.23
ethylbenzene	CCc1ccccc1	toluene		-5.93	-10.14	-10.25
anisole	COc1ccccc1	toluene		-6.04	-11.10	-10.34
3-methylphenol	Cc1cccc(O)c1	toluene		-6.72	-12.25	-11.80
acetophenone	CC(=O)c1ccccc1	toluene		-7.28	-12.56	-12.39
acetonitrile	CC#N	toluene		-3.61	-7.46	-6.03
ethyl acetate	CCOC(C)=O	toluene		-4.40	-8.34	-7.96
propyl acetate	CCCOC(C)=O	toluene		-5.13	-9.39	-9.13
ethyl propanoate	CCOC(=O)CC	toluene		-5.04	-9.46	-8.95
propyl propanoate	CCCOC(=O)CC	toluene		-5.73	-10.51	-10.10
2-chlorotoluene	Cc1ccccc1Cl	toluene		-6.37	-11.06	-10.84
benzaldehyde	O=Cc1ccccc1	toluene		-6.46	-11.70	-10.99
pyrrole	[nH]1ccccc1	toluene		-4.86	-9.92	-8.45
γ butyrolactone	O=C1CCCO1	toluene		-5.88	-12.48	-10.66
tridecane	CCCCCCCCCCCCC	chloroform		-8.34	-14.35	-14.52
pentadecane	CCCCCCCCCCCCCCC	chloroform		-9.81	-16.19	-16.80
hexadecane	CCCCCCCCCCCCCCCC	chloroform		-10.43	-17.67	-17.77
toluene	Cc1ccccc1	chloroform		-5.17	-9.82	-9.19
1,4-dimethylbenzene	Cc1ccc(C)cc1	chloroform		-5.78	-11.04	-10.13
anthracene	c1ccc2cc3ccccc3cc2c1	chloroform		-11.06	-18.75	-18.45
dipropyl ether	CCCOCC	chloroform		-5.23	-10.09	-9.52
diisopropyl ether	CC(C)OC(C)C	chloroform		-4.80	-9.87	-8.89
dibutyl ether	CCCCOCCCC	chloroform		-6.55	-12.19	-11.67
1,3-dioxane	C1COCOC1	chloroform		-5.05	-11.52	-9.09
methyl ethyl ketone	CCC(C)=O	chloroform		-4.67	-10.40	-8.49
5-nonanone	CCCCC(=O)CCCC	chloroform		-8.03	-15.12	-14.00
ethyl propanoate	CCOC(=O)CC	chloroform		-5.52	-11.69	-9.94
propyl benzoate	CCCOC(=O)c1ccccc1	chloroform		-9.34	-17.11	-15.82
butyl benzoate	CCCCOC(=O)c1ccccc1	chloroform		-10.06	-18.09	-16.99
3-methylpyridine	Cc1ccnc1	chloroform		-6.82	-13.21	-11.55
nitromethane	C[N+](=O)[O-]	chloroform		-4.44	-9.01	-8.43
methanol	CO	chloroform		-2.69	-6.86	-5.79
1-hexanol	CCCCCCO	chloroform		-6.31	-12.05	-11.76
1-chloroheptane	CCCCCCCCl	chloroform		-6.65	-11.71	-11.81
1-chlorooctane	CCCCCCCCCl	chloroform		-7.24	-12.78	-12.76
octane	CCCCCCCC	tert-butanol		-5.14	-8.55	-9.65
nonane	CCCCCCCCC	tert-butanol		-5.78	-9.63	-10.59
decane	CCCCCCCCC	tert-butanol		-6.44	-10.67	-11.64
triethylamine	CCN(CC)CC	tert-butanol		-4.52	-9.15	-9.06
benzene	c1ccccc1	tert-butanol		-4.31	-6.24	-7.69
1,2-dimethylbenzene	Cc1ccccc1C	tert-butanol		-5.45	-9.06	-9.46
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	tert-butanol		-6.00	-9.33	-10.28
2-ethoxyethanol	CCOCCO	tert-butanol		-6.21	-11.29	-12.20
ethanediol	CC(O)O	tert-butanol		-5.54	-14.60	-12.86
glycerol	OC(CO)CO	tert-butanol		-6.66	-20.51	-15.61
dimethyl ether	COC	tert-butanol		-2.25	-3.97	-4.37
5-nonanone	CCCCC(=O)CCCC	tert-butanol		-7.44	-11.87	-12.69
di-tert-butylketone	CC(C)(C)C(=O)C(C)(C)C	tert-butanol		-5.83	-9.40	-10.28
propyl formate	CCCOC=O	tert-butanol		-4.03	-7.04	-6.91
propyl acetate	CCCOC(C)=O	tert-butanol		-4.61	-7.77	-7.87
propyl propanoate	CCCOC(=O)CC	tert-butanol		-5.28	-8.95	-9.07
ethyl butanoate	CCCC(=O)OCC	tert-butanol		-5.36	-8.37	-9.21
butyl butanoate	CCCCOC(=O)CCC	tert-butanol		-6.64	-10.81	-11.40
acetonitrile	CC#N	tert-butanol		-4.33	-5.26	-7.01
1-bromobutane	CCCCBr	tert-butanol		-4.25	-5.76	-7.79
heptane	CCCCCCC	2-methyl-2-butanol		-4.56	-8.20	-8.64
2-methyl-2-butanol	CCC(C)(C)O	2-methyl-2-butanol		-4.97	-11.97	-10.28
1-bromoadamantane	BrC12CC3CC(C(C3)C1)C2	2-methyl-2-butanol		-8.11	-12.81	-12.93
2-methyl-2-bromopropane	CC(C)(C)Br	2-methyl-2-butanol		-3.79	-6.36	-7.07

1-butylamine	CCCCN	2-methyl-2-butanol		-5.12	-10.47	-10.46
1-heptylamine	CCCCCCCN	2-methyl-2-butanol		-6.77	-13.93	-13.35
octane	CCCCCCCC	diethyl ether		-5.36	-9.46	-9.62
methanol	CO	diethyl ether		-3.68	-8.03	-8.17
1-nitropropane	CCC[N+](=O)[O-]	diethyl ether		-5.21	-10.29	-9.67
1-chlorobutane	CCCCl	diethyl ether		-4.37	-8.14	-8.20
4-fluoroanisole	COc1ccc(F)cc1	diethyl ether		-6.69	-11.99	-11.92
tetramethylstannane	C[Sn](C)(C)C	diethyl ether		-4.16	-6.97	-6.60
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	diethyl ether		-6.48	-11.22	-11.33
hexane	CCCCCC	dibutyl ether		-3.93	-7.44	-7.76
decane	CCCCCCCCC	dibutyl ether		-6.73	-12.10	-12.14
3-methylpentane	CCC(C)CC	dibutyl ether		-3.77	-7.17	-7.48
cyclohexane	C1CCCCC1	dibutyl ether		-4.10	-7.74	-7.61
1-octyne	CCCCCCC#C	dibutyl ether		-5.33	-10.33	-9.63
2-octyne	CCCCC#CC	dibutyl ether		-5.28	-10.72	-9.53
benzene	c1ccccc1	dibutyl ether		-4.22	-7.90	-7.95
toluene	Cc1ccccc1	dibutyl ether		-4.92	-9.05	-9.07
3-methyl-1-butanol	CC(C)CCO	dibutyl ether		-5.63	-11.39	-11.44
diethyl ether	CCOCC	dibutyl ether		-3.39	-6.38	-6.75
dibutyl ether	CCCOCCCC	dibutyl ether		-6.06	-10.76	-10.88
nonan-2-one	CCCCCCCC(C)=O	dibutyl ether		-7.07	-12.89	-12.35
nonan-5-one	CCCCC(=O)CCCC	dibutyl ether		-6.87	-12.27	-12.01
butylamine	CCCCN	dibutyl ether		-4.44	-7.88	-9.06
triethylamine	CCN(CC)CC	dibutyl ether		-4.45	-8.50	-8.74
acetonitrile	CC#N	dibutyl ether		-2.85	-6.40	-4.87
aniline	Nc1ccccc1	dibutyl ether		-7.18	-13.06	-13.39
1,1,2,2-tetrachloroethane	ClC(Cl)C(Cl)Cl	dibutyl ether		-6.36	-11.98	-11.37
pentanoic acid	CCCCC(O)=O	dibutyl ether		-6.62	-14.78	-13.39
pyrrole	[nH]1ccccc1	dibutyl ether		-5.50	-11.63	-10.45
heptane	CCCCCCC	ethyl acetate		-4.12	-7.14	-7.41
octane	CCCCCCCC	ethyl acetate		-4.67	-8.09	-8.17
nonane	CCCCCCCCC	ethyl acetate		-5.40	-8.99	-9.35
tridecane	CCCCCCCCCCCCC	ethyl acetate		-7.80	-13.53	-12.94
hexadecane	CCCCCCCCCCCCCCCC	ethyl acetate		-9.92	-15.98	-16.25
cyclohexane	C1CCCCC1	ethyl acetate		-3.86	-6.54	-6.73
acetone	CC(C)=O	ethyl acetate		-3.66	-7.36	-7.11
4-heptanone	CCCC(=O)CCC	ethyl acetate		-6.32	-10.61	-11.20
di-tert-butylketone	CC(C)(C)C(=O)C(C)(C)C	ethyl acetate		-6.14	-10.34	-10.87
1-butanol	CCCCO	ethyl acetate		-5.43	-10.37	-11.02
2-methyl-2-butanol	CCC(C)(C)O	ethyl acetate		-4.69	-9.87	-9.48
butyl methyl ether	CCCCOC	ethyl acetate		-4.19	-7.36	-7.57
18-crown-6	C1COCOCOCOCOCOCOC1	ethyl acetate		-12.00	-23.57	-21.79
1-fluorooctane	CCCCCCCCF	ethyl acetate		-6.04	-11.15	-10.69
tetrachloroethene	ClC(Cl)=C(Cl)Cl	ethyl acetate		-5.28	-9.09	-9.74
benzene	c1ccccc1	ethyl acetate		-4.41	-8.00	-7.90
toluene	Cc1ccccc1	ethyl acetate		-4.93	-8.96	-8.66
ethyl pentanoate	CCCCC(=O)OCC	ethyl acetate		-6.45	-11.12	-11.42
sulfur dioxide	O=[S]=O	ethyl acetate		-3.52	-7.10	-8.06
piperidine	C1CCNCC1	ethyl acetate		-5.78	-9.44	-10.44
diethyl malonate	CCOC(=O)CC(=O)OCC	ethyl acetate		-8.25	-15.46	-14.39
N,N-dimethylacetamide	CN(C)C(C)=O	ethyl acetate		-6.70	-12.24	-12.49
water	O	ethyl acetate		-4.34	-8.56	-10.53
N-methylimidazole	Cn1ccnc1	ethyl acetate		-7.52	-12.70	-12.95
trans-1,2-dichloroethene	ClC=C(Cl)	dimethyl carbonate		-3.78	-7.24	-7.29
propan-1-ol	CCCO	dimethyl carbonate		-3.84	-8.63	-8.26
2-butanol	CCC(C)O	dimethyl carbonate		-4.10	-8.80	-8.49
2-methyl-isopropanol	CC(C)(C)O	dimethyl carbonate		-3.53	-8.30	-7.57
diethyl carbonate	CCOC(=O)OCC	dimethyl carbonate		-5.03	-10.42	-9.55
acetone	CC(C)=O	dimethyl carbonate		-3.26	-7.28	-6.66
2-pentanone	CCCC(C)=O	dimethyl carbonate		-4.76	-8.79	-9.01
propyl acetate	CCCOC(C)=O	dimethyl carbonate		-5.04	-8.72	-9.60
butyl acetate	CCCCOC(C)=O	dimethyl carbonate		-5.63	-10.12	-10.47
pentyl acetate	CCCCCOC(C)=O	dimethyl carbonate		-6.26	-11.31	-11.41
ethylbenzene	CCc1ccccc1	dimethyl carbonate		-5.50	-9.38	-9.71
1,3-dimethylbenzene	Cc1cccc(C)c1	dimethyl carbonate		-5.51	-9.50	-9.79
1,1,1,2-tetrafluoroethane	FCF(F)(F)F	dimethyl carbonate		-0.69	-4.68	-1.50
2-phenylethanol	OCCc1ccccc1	dimethyl carbonate		-7.94	-15.94	-14.65
p-cymene	CC(C)c1ccc(C)cc1	dimethyl carbonate		-6.81	-10.93	-11.77
propanoic acid	CCC(O)=O	dimethyl carbonate		-5.22	-12.31	-11.21
krypton	[Kr]	diethyl carbonate		0.43	-0.63	-0.41
carbon dioxide	O=C=O	diethyl carbonate		-0.46	-2.85	-2.68
methane	C	diethyl carbonate		0.37	-0.43	-0.55
hexan-1-ol	CCCCCCO	diethyl carbonate		-5.68	-11.78	-11.26
2-pentanol	CCCC(C)O	diethyl carbonate		-4.77	-10.31	-9.78
3-pentanol	CCC(O)CC	diethyl carbonate		-4.77	-10.03	-9.83
2-methyl-1-butanol	CCC(C)CO	diethyl carbonate		-4.89	-10.37	-10.05
3-methyl-2-butanol	CC(C)(C)CO	diethyl carbonate		-4.54	-9.80	-9.43
dimethyl carbonate	COC(=O)OC	diethyl carbonate		-4.21	-8.94	-8.66
propyl acetate	CCCOC(C)=O	diethyl carbonate		-4.99	-9.49	-9.75
pentyl acetate	CCCCCOC(C)=O	diethyl carbonate		-6.25	-11.11	-11.66
hexyl acetate	CCCCCOC(C)=O	diethyl carbonate		-6.89	-12.28	-12.60
1,3-dimethylbenzene	Cc1cccc(C)c1	diethyl carbonate		-5.39	-10.09	-9.77
benzyl alcohol	OCc1ccccc1	diethyl carbonate		-7.31	-13.79	-13.95

phenetole	CCOc1ccccc1	diethyl carbonate		-6.66	-12.01	-12.00
hexane	CCCCCC	acetic acid		-3.09	-6.19	-6.50
2,3-dimethylpentane	CCC(C)C(C)C	acetic acid		-3.40	-7.01	-7.00
cyclopentane	C1CCCC1	acetic acid		-2.77	-5.65	-5.55
cycloheptane	C1CCCCC1	acetic acid		-4.20	-7.66	-7.83
1-methylcyclopentene	CC1=CCCC1	acetic acid		-3.71	-7.00	-7.15
cyclooctene	C1CCCC=CCC1	acetic acid		-5.60	-8.64	-10.75
cyclohepta-1,3,5-triene	C1C=CC=CC=C1	acetic acid		-4.81	-8.62	-9.02
methanol	CO	acetic acid		-3.22	-8.77	-8.08
pentan-1-ol	CCCCCO	acetic acid		-5.99	-12.91	-12.68
methyl acetate	COC(C)=O	acetic acid		-3.40	-7.86	-6.85
ethyl butanoate	CCCC(=O)OCC	acetic acid		-5.41	-10.31	-10.25
tetrahydrofuran	C1CCOC1	acetic acid		-3.47	-8.60	-6.59
1,3-dioxolane	C1COCO1	acetic acid		-3.61	-8.38	-7.09
<i>o</i> -xylene	Cc1ccccc1C	acetic acid		-5.52	-9.67	-10.31
krypton	[Kr]	chlorobenzene		0.12	-0.73	-0.81
ethane	CC	chlorobenzene		-0.64	-2.36	-1.95
propane	CCC	chlorobenzene		-1.32	-3.77	-2.97
<i>n</i> -octane	CCCCCCCC	chlorobenzene		-4.74	-9.18	-8.45
<i>n</i> -decane	CCCCCCCCC	chlorobenzene		-6.34	-11.42	-11.04
<i>n</i> -dodecane	CCCCCCCCCCCC	chlorobenzene		-7.69	-13.65	-13.25
<i>n</i> -hexadecane	CCCCCCCCCCCCCCCC	chlorobenzene		-10.11	-18.05	-17.38
cyclohexane	C1CCCCC1	chlorobenzene		-4.10	-7.31	-7.27
trichloromethane	ClC(Cl)Cl	chlorobenzene		-4.32	-7.58	-7.74
tetrahydropyran	C1CCOCC1	chlorobenzene		-5.19	-9.53	-9.18
heptan-2-one	CCCCCCC(=O)	chlorobenzene		-6.76	-11.72	-11.80
octan-2-one	CCCCCCC(=O)C	chlorobenzene		-7.57	-12.77	-13.10
methyl acetate	COC(C)=O	chlorobenzene		-4.55	-7.68	-8.10
ethyl acetate	CCOC(C)=O	chlorobenzene		-4.91	-8.55	-8.70
methyl salicylate	COC(=O)c1ccccc1O	chlorobenzene		-9.19	-13.45	-15.91
ethyl salicylate	CCOC(=O)c1ccccc1O	chlorobenzene		-10.04	-14.89	-18.17
methyl benzoate	COC(=O)c1ccccc1	chlorobenzene		-8.12	-13.46	-13.55
benzonitrile	N#Cc1ccccc1	chlorobenzene		-8.41	-11.85	-13.27
<i>o</i> -xylene	Cc1ccccc1C	chlorobenzene		-6.03	-10.48	-10.58
<i>m</i> -xylene	Cc1ccc(C)cc1	chlorobenzene		-6.06	-10.31	-10.60
1,3,5-trimethylbenzene	Cc1cc(C)cc(C)c1	chlorobenzene		-6.62	-11.37	-11.46
1,2-dichlorobenzene	Clc1ccccc1Cl	chlorobenzene		-6.98	-11.79	-11.91
pyrrole	[nH]1cccc1	chlorobenzene		-5.72	-9.61	-9.90
2-methylpyridine	Cc1ccccn1	chlorobenzene		-6.67	-10.38	-11.16
4-methylpyridine	Cc1ccncc1	chlorobenzene		-6.66	-10.69	-11.05
2,4-dimethylpyridine	Cc1ccnc(C)c1	chlorobenzene		-7.47	-11.60	-12.54
2,6-dimethylpyridine	Cc1ccc(C)nn1	chlorobenzene		-7.44	-11.14	-12.59
tetramethylstannane	C[Sn](C)(C)C	chlorobenzene		-3.86	-7.34	-6.56
<i>n</i> -methylpyrazole	Cn1cccn1	chlorobenzene		-5.77	-10.64	-9.75
isoquinoline	c1ccc2ncccc2c1	chlorobenzene		-9.44	-14.41	-15.41
ethylcyclohexane	CCC1CCCCC1	formamide		-3.39	-7.30	-7.66
1-heptene	CCCCCC=C	formamide		-2.61	-7.20	-6.41
<i>cis</i> -2-hexene	CCC/C=C/C	formamide		-2.08	-6.20	-5.56
cyclohexene	C1CCC=CC1	formamide		-2.80	-6.30	-6.63
1-propanol	CCCO	formamide		-4.20	-10.62	-11.09
isopropanol	CC(C)O	formamide		-3.79	-10.10	-10.45
isobutanol	CC(C)CO	formamide		-4.52	-11.37	-11.55
2-methyl-isopropanol	CC(C)(C)O	formamide		-3.80	-10.46	-10.31
octan-1-ol	CCCCCCCCO	formamide		-6.61	-15.06	-14.76
1,4-butanediol	OCCCCO	formamide		-8.22	-18.26	-19.45
1,3-dioxolane	C1COCO1	formamide		-4.10	-8.56	-8.99
toluene	Cc1ccccc1	formamide		-3.70	-8.01	-8.01
fluorobenzene	Fc1ccccc1	formamide		-3.63	-7.46	-8.03
biphenyl	c1ccc(cc1)c2ccccc2	formamide		-7.69	-13.77	-13.91
<i>N</i> -ethylformamide	CCNC=O	formamide		-6.78	-14.26	-14.62
<i>N</i> -ethylacetamide	CCNC(C)=O	formamide		-7.22	-15.78	-16.05
urea	NC(N)=O	formamide		-4.89	-17.83	-8.12
phenol	Oc1ccccc1	formamide		-6.72	-14.34	-14.27
2-methylbutane	CCC(C)C	methylformamide		-1.89	-4.38	-4.19
chlorobenzene	Clc1ccccc1	methylformamide		-5.35	-9.54	-9.91
methanol	CO	methylformamide		-4.08	-8.38	-9.61
1,4-butanediol	OCCCCO	methylformamide		-7.78	-18.28	-16.74
acetone	CC(C)=O	methylformamide		-4.11	-7.08	-8.22
3-nitrophenol	Oc1cccc(c1)[N+](=O)[O-]	methylformamide		-11.67	-21.92	-22.13
4-chlorophenol	Oc1ccc(Cl)cc1	methylformamide		-8.95	-18.38	-17.36
formamide	NC=O	methylformamide		-5.88	-15.25	-12.15
hexadecane	CCCCCCCCCCCCCCCC	triethylamine		-10.86	-19.10	-18.34
methyl ethyl ketone	CCC(C)=O	triethylamine		-3.71	-7.20	-7.14
diethyl ether	CCOCC	triethylamine		-3.52	-6.48	-6.90
1-pentanol	CCCCCO	triethylamine		-5.36	-14.65	-10.70
2-methyl-2-butanol	CCC(C)(C)O	triethylamine		-4.49	-12.01	-9.18
toluene	Cc1ccccc1	triethylamine		-4.97	-8.95	-9.10
anisole	COc1ccccc1	triethylamine		-5.69	-10.44	-10.15
<i>N</i> -methylpyrrole	Cn1cccc1	triethylamine		-4.87	-8.86	-8.88
<i>N</i> -methylimidazole	Cn1ccnc1	triethylamine		-6.19	-10.88	-10.92
dimethylformamide	CN(C)C=O	triethylamine		-5.14	-9.27	-10.07
octane	CCCCCCCC	benzotrifluoride		-4.81	-8.91	-8.34
2-methylbutane	CCC(C)C	benzotrifluoride		-2.82	-5.31	-5.40

2,2,4,4-tetramethylpentane	CC(C)(C)CC(C)(C)C	benzotrifluoride		-4.42	-8.26	-8.03
methyl <i>tert</i> -butyl ether	COC(C)(C)C	benzotrifluoride		-4.43	-6.93	-8.25
acetone	CC(C)=O	benzotrifluoride		-4.50	-7.53	-8.62
1-pentanol	CCCCCO	benzotrifluoride		-5.53	-9.29	-10.64
toluene	Cc1ccccc1	benzotrifluoride		-5.11	-9.03	-8.80
anisole	COc1ccccc1	benzotrifluoride		-6.66	-10.95	-11.45
argon	[Ar]	ethylene glycol		1.22	-0.22	0.14
hydrogen	[H][H]	ethylene glycol		1.51	1.41	0.49
methylcyclohexane	CC1CCCCC1	ethylene glycol		-3.33	-6.55	-7.79
1,4-dioxane	C1COCCO1	ethylene glycol		-4.71	-8.39	-10.14
2-pentanone	CCCC(C)=O	ethylene glycol		-4.13	-8.08	-8.87
butyl acetate	CCCCOC(C)=O	ethylene glycol		-4.51	-9.11	-9.54
isopropanol	CC(C)O	ethylene glycol		-4.08	-10.33	-10.89
benzene	c1ccccc1	ethylene glycol		-3.42	-7.60	-7.69
ethylbenzene	CCc1ccccc1	ethylene glycol		-4.57	-9.30	-9.42
<i>o</i> -xylene	Cc1ccccc1C	ethylene glycol		-4.49	-9.39	-9.37
2-methylpyridine	Cc1ccccc1	ethylene glycol		-5.99	-11.78	-11.66
3-methylpyridine	Cc1ccccc1	ethylene glycol		-6.03	-11.93	-11.68
4-methylpyridine	Cc1ccccc1	ethylene glycol		-6.01	-12.14	-11.61
acetic acid	CC(O)=O	ethylene glycol		-5.68	-12.28	-13.33
sec-butylamine	CCC(C)N	ethylene glycol		-4.16	-11.74	-11.83
<i>tert</i> -butylamine	CC(C)(C)N	ethylene glycol		-4.08	-11.90	-12.05
diethylamine	CCNCC	ethylene glycol		-3.71	-11.64	-10.31
<i>n</i> -hexane	CCCCCC	pyridine		-3.30	-5.93	-6.15
<i>n</i> -decane	CCCCCCCCC	pyridine		-6.12	-9.89	-10.67
1,3,5-tribromobenzene	Br1cc(Br)cc(Br)c1	pyridine		-9.90	-15.15	-16.71
3-nitrophenol	Oc1cccc(c1)[N+](=O)[O-]	pyridine		-11.74	-21.75	-21.69
4-bromophenol	Oc1ccc(Br)cc1	pyridine		-10.36	-21.15	-19.16
ethyl-2-hydroxybenzoate	CCOC(=O)c1ccccc1O	pyridine		-10.23	-14.48	-18.78
1,4-dihydroxybenzene	Oc1ccc(O)cc1	pyridine		-11.86	-25.33	-23.01
acetophenone	CC(=O)c1ccccc1	pyridine		-8.13	-13.31	-13.67
<i>N</i> -methylimidazole	Cn1ccnc1	pyridine		-7.46	-12.26	-12.50
pyrazole	[nH]1cccn1	pyridine		-7.05	-15.27	-12.57
1,2-diazine	c1ccnnc1	pyridine		-5.58	-12.72	-8.73
formamide	NC=O	pyridine		-7.80	-15.06	-15.33
$\delta$ -valerolactam	O=C1CCCCN1	pyridine		-9.51	-16.90	-17.18
<i>n</i> -methylcaprolactam	CN1CCCCC1=O	pyridine		-8.94	-15.65	-15.80
decane	CCCCCCCCC	methyl acetate		-5.97	-9.46	-10.06
tridecane	CCCCCCCCCCCC	methyl acetate		-7.73	-12.01	-12.68
1-chloropentane	CCCCCl	methyl acetate		-4.67	-8.39	-8.40
1,2-dichloropropane	CC(Cl)CCl	methyl acetate		-5.12	-8.78	-9.06
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	methyl acetate		-5.36	-7.63	-9.48
1,3-dibromopropane	BrCCCB	methyl acetate		-6.27	-11.26	-11.06
ethanol	CCO	methyl acetate		-4.27	-8.33	-9.17
butylbenzene	CCCCc1ccccc1	methyl acetate		-6.89	-11.24	-11.48
1,2-dichloroethane	C1CCCl	methyl ethyl ketone		-4.45	-7.75	-7.90
1-pentanol	CCCCCO	methyl ethyl ketone		-6.15	-12.17	-12.08
1-octanol	CCCCCCCCO	methyl ethyl ketone		-8.14	-15.11	-15.19
1-decanol	CCCCCCCCCO	methyl ethyl ketone		-9.16	-17.24	-16.93
2-octanone	CCCCCCC(C)=O	methyl ethyl ketone		-6.82	-12.18	-11.53
toluene	Cc1ccccc1	methyl ethyl ketone		-4.84	-9.13	-8.42
1-methylnaphthalene	Cc1cccc2ccccc12	methyl ethyl ketone		-8.15	-14.58	-13.66
hexane	CCCCCC	nitromethane		-2.48	-4.27	-4.76
2-methylpentane	CCCC(C)C	nitromethane		-2.27	-3.82	-4.43
dichloromethane	C1CCl	nitromethane		-3.26	-6.44	-6.17
1-chloropropane	CCCl	nitromethane		-3.28	-5.61	-6.33
1-propanol	CCCO	nitromethane		-4.47	-8.03	-9.50
nitroethane	CC[N+](=O)[O-]	nitromethane		-5.44	-9.81	-10.18
benzene	c1ccccc1	nitromethane		-4.03	-7.06	-7.20
toluene	Cc1ccccc1	nitromethane		-4.64	-7.86	-8.18
<i>p</i> -xylene	Cc1ccc(C)cc1	nitromethane		-5.21	-8.53	-9.10
hexane	CCCCCC	<i>N</i> -methyl-2-pyrrolidone		-2.43	-5.65	-5.43
octane	CCCCCCCC	<i>N</i> -methyl-2-pyrrolidone		-3.52	-7.34	-7.26
cyclopentene	C1CC=CC1	<i>N</i> -methyl-2-pyrrolidone		-3.01	-5.00	-6.33
1-chlorohexane	CCCCCCl	<i>N</i> -methyl-2-pyrrolidone		-5.17	-9.68	-9.90
acetone	CC(C)=O	<i>N</i> -methyl-2-pyrrolidone		-3.45	-6.79	-6.93
2-pentanone	CCCC(C)=O	<i>N</i> -methyl-2-pyrrolidone		-4.57	-8.78	-8.64
3-pentanone	CCC(=O)CC	<i>N</i> -methyl-2-pyrrolidone		-4.54	-8.42	-8.54
ethyl propanoate	CCOC(=O)CC	<i>N</i> -methyl-2-pyrrolidone		-4.46	-8.82	-8.48
ethyl butyrate	CCCC(=O)OCC	<i>N</i> -methyl-2-pyrrolidone		-4.84	-9.28	-9.19
benzene	c1ccccc1	<i>N</i> -methyl-2-pyrrolidone		-3.84	-7.38	-7.47
anthracene	c1ccc2cc3ccccc3cc2c1	<i>N</i> -methyl-2-pyrrolidone		-10.70	-20.23	-18.38
<i>m</i> -terphenyl	c1ccc(cc1)c2ccccc2c3ccccc3	<i>N</i> -methyl-2-pyrrolidone		-13.42	-24.79	-21.93
1-naphthol	Oc1ccc2ccccc12	<i>N</i> -methyl-2-pyrrolidone		-10.97	-23.42	-20.32
methylformamide	CNC=O	<i>N</i> -methyl-2-pyrrolidone		-6.65	-13.77	-13.18
octane	CCCCCCCC	2-methoxyethanol		-4.00	-7.84	-7.66
nonane	CCCCCCCCC	2-methoxyethanol		-4.85	-8.77	-9.07
undecane	CCCCCCCCCCC	2-methoxyethanol		-6.17	-10.66	-11.23
cyclohexane	C1CCCCC1	2-methoxyethanol		-3.21	-6.36	-5.97
toluene	Cc1ccccc1	2-methoxyethanol		-4.54	-8.80	-8.35
ethylbenzene	CCc1ccccc1	2-methoxyethanol		-5.23	-9.68	-9.38
2-methoxyethanol	COCCO	2-methoxyethanol		-5.25	-10.80	-11.41
hexane	CCCCCC	propylene glycol		-2.32	-6.12	-5.92

octane	CCCCCCCC	propylene glycol	-3.47	-8.20	-7.80
decane	CCCCCCCCC	propylene glycol	-5.10	-10.28	-10.47
<i>o</i> -xylene	Cc1ccccc1C	propylene glycol	-4.58	-9.23	-9.18
biphenyl	c1ccc(cc1)c2ccccc2	propylene glycol	-8.34	-14.27	-14.77
2-chloro-2-methylpropane	CC(C)(C)Cl	propylene glycol	-2.96	-5.80	-6.81
2-chloro-2-methylbutane	CCC(C)(C)Cl	propylene glycol	-3.62	-7.04	-7.86
3-chloro-3-methylpentane	CCC(C)(Cl)CC	propylene glycol	-4.22	-8.22	-8.84
chlorobenzene	Clc1ccccc1	cyclohexanone	-5.41	-10.27	-9.46
toluene	Cc1ccccc1	cyclohexanone	-4.70	-9.23	-8.44
neon	[Ne]	cyclohexanone	1.94	2.10	1.86
argon	[Ar]	cyclohexanone	1.06	0.16	0.32
methyl ethyl ketone	CCC(C)=O	cyclohexanone	-3.95	-8.24	-7.01
diethyl carbonate	CCOC(=O)OCC	cyclohexanone	-4.75	-10.14	-8.32
<i>N</i> -methylimidazole	Cn1ccnc1	cyclohexanone	-6.98	-12.68	-11.77
neon	[Ne]	2-methyltetrahydrofuran	1.95	0.39	1.88
argon	[Ar]	2-methyltetrahydrofuran	0.69	-0.58	0.04
hydrogen	[H][H]	2-methyltetrahydrofuran	1.30	0.57	0.84
nitrogen	N#N	2-methyltetrahydrofuran	0.86	-0.05	0.58
carbon tetrafluoride	FC(F)(F)F	2-methyltetrahydrofuran	0.95	-0.25	0.32
benzene	c1ccccc1	2-methyltetrahydrofuran	-4.73	-8.28	-8.48
chlorobenzene	Clc1ccccc1	2-methyltetrahydrofuran	-5.91	-10.42	-10.29

**Table S4.** ESE-ΔH-DNN solvation free energies of nonpolar solvents from MNSol database (Marenich, A. V.; Kelly, C. P.; Thompson, J. D.; Hawkins, G. D.; Chambers, C. C.; Giesen, D. J.; Winget, P.; Cramer, C. J.; Truhlar D. G., Minnesota Solvation Database – version 2012, University of Minnesota, November 26, 2012. [https://conservancy.umn.edu/bitstream/handle/11299/213300/MNSolDatabase\\_v2012.zip](https://conservancy.umn.edu/bitstream/handle/11299/213300/MNSolDatabase_v2012.zip))

Solute code	Solvent	Formula	ΔG <sub>sol</sub> <sup>o</sup> (exp)	ΔG <sub>sol</sub> <sup>o</sup> (calc)
0005npe	pentane	C <sub>5</sub> H <sub>12</sub>	-3.35	-3.37
0044met	pentane	CH <sub>4</sub> O	-1.29	-1.71
0045eth	pentane	C <sub>2</sub> H <sub>6</sub> O	-2.15	-2.56
0047pro	pentane	C <sub>3</sub> H <sub>8</sub> O	-2.76	-3.28
0049but	pentane	C <sub>4</sub> H <sub>10</sub> O	-3.77	-4.03
0052pen	pentane	C <sub>3</sub> H <sub>12</sub> O	-3.92	-4.68
0053phe	pentane	C <sub>6</sub> H <sub>6</sub> O	-5.67	-5.39
0054hex	pentane	C <sub>6</sub> H <sub>14</sub> O	-4.97	-5.42
0058hep	pentane	C <sub>7</sub> H <sub>16</sub> O	-5.62	-6.17
0078pen	pentane	C <sub>3</sub> H <sub>10</sub> O	-4.16	-4.57
0080hex	pentane	C <sub>6</sub> H <sub>12</sub> O	-4.79	-5.25
0081dim	pentane	C <sub>6</sub> H <sub>12</sub> O	-4.43	-4.52
0082hep	pentane	C <sub>7</sub> H <sub>14</sub> O	-5.40	-5.93
0093met	pentane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.13	-3.46
0094met	pentane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.69	-4.07
0095eth	pentane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.69	-3.99
0097pro	pentane	C <sub>3</sub> H <sub>10</sub> O <sub>2</sub>	-4.21	-4.62
0098met	pentane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.96	-5.40
0099but	pentane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.88	-5.28
0100met	pentane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.67	-6.06
0101pen	pentane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.62	-5.95
0103eth	pentane	C <sub>2</sub> H <sub>7</sub> N	-2.18	-2.62
0106pro	pentane	C <sub>3</sub> H <sub>9</sub> N	-3.13	-3.33
0118ani	pentane	C <sub>6</sub> H <sub>7</sub> N	-5.15	-6.00
0162tri	pentane	CHCl <sub>3</sub>	-3.26	-3.67
0179tri	pentane	CHBr <sub>3</sub>	-4.83	-5.87
0006nhe	hexane	C <sub>6</sub> H <sub>14</sub>	-4.00	-3.99
0008noc	hexane	C <sub>8</sub> H <sub>18</sub>	-5.46	-5.43
0035ben	hexane	C <sub>6</sub> H <sub>6</sub>	-3.96	-4.28
0036tol	hexane	C <sub>7</sub> H <sub>8</sub>	-4.84	-4.84
0037eth	hexane	C <sub>8</sub> H <sub>10</sub>	-4.99	-5.52
0038oxy	hexane	C <sub>8</sub> H <sub>10</sub>	-5.22	-5.40
0039mxy	hexane	C <sub>8</sub> H <sub>10</sub>	-4.99	-5.39
0040pxy	hexane	C <sub>8</sub> H <sub>10</sub>	-5.01	-5.39
0044met	hexane	CH <sub>4</sub> O	-1.49	-1.59
0045eth	hexane	C <sub>2</sub> H <sub>6</sub> O	-2.73	-2.42
0047pro	hexane	C <sub>3</sub> H <sub>8</sub> O	-2.81	-3.14
0049but	hexane	C <sub>4</sub> H <sub>10</sub> O	-3.77	-3.89
0052pen	hexane	C <sub>3</sub> H <sub>12</sub> O	-4.38	-4.55
0053phe	hexane	C <sub>6</sub> H <sub>6</sub> O	-5.49	-5.26
0054hex	hexane	C <sub>6</sub> H <sub>14</sub> O	-5.14	-5.28
0055ocr	hexane	C <sub>7</sub> H <sub>8</sub> O	-6.25	-5.95
0057per	hexane	C <sub>7</sub> H <sub>8</sub> O	-5.86	-5.97
0058hep	hexane	C <sub>7</sub> H <sub>16</sub> O	-5.75	-6.02
0062dio	hexane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.08	-4.34
0074ben	hexane	C <sub>7</sub> H <sub>6</sub> O	-5.53	-5.70
0075pro	hexane	C <sub>3</sub> H <sub>6</sub> O	-2.60	-2.83
0076but	hexane	C <sub>4</sub> H <sub>8</sub> O	-3.48	-3.70
0080hex	hexane	C <sub>6</sub> H <sub>12</sub> O	-4.68	-5.07
0081dim	hexane	C <sub>6</sub> H <sub>12</sub> O	-4.34	-4.33
0082hep	hexane	C <sub>7</sub> H <sub>14</sub> O	-5.36	-5.75
0084met	hexane	C <sub>8</sub> H <sub>8</sub> O	-6.05	-6.33
0086eth	hexane	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-2.83	-2.90
0087pro	hexane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-2.98	-3.65

0093met	hexane	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	-3.12	-3.26
0094met	hexane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.65	-3.89
0095eth	hexane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.62	-3.79
0097pro	hexane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.10	-4.43
0098met	hexane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.94	-5.21
0099but	hexane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.86	-5.10
0100met	hexane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.64	-5.88
0101pen	hexane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.52	-5.77
0103eth	hexane	C <sub>2</sub> H <sub>7</sub> N	-2.09	-2.42
0106pro	hexane	C <sub>3</sub> H <sub>9</sub> N	-3.13	-3.15
0110but	hexane	C <sub>4</sub> H <sub>11</sub> N	-3.62	-3.89
0116pyr	hexane	C <sub>5</sub> H <sub>5</sub> N	-3.81	-4.84
0118ani	hexane	C <sub>6</sub> H <sub>7</sub> N	-5.43	-5.86
0130nit	hexane	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	-3.19	-3.29
0133nit	hexane	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	-4.64	-4.85
0134nit	hexane	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-6.09	-6.00
0151phy	hexane	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-9.18	-6.74
0157flu	hexane	C <sub>6</sub> H <sub>5</sub> F	-4.15	-4.40
0162tri	hexane	CHCl <sub>3</sub>	-3.17	-3.65
0174chl	hexane	C <sub>6</sub> H <sub>5</sub> Cl	-5.14	-5.31
0176pdi	hexane	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-5.69	-6.35
0179tri	hexane	CHBr <sub>3</sub>	-4.38	-5.70
0186bro	hexane	C <sub>6</sub> H <sub>5</sub> Br	-5.66	-5.66
0215pbr	hexane	C <sub>6</sub> H <sub>5</sub> OBr	-6.96	-7.33
0220tri	hexane	C <sub>3</sub> H <sub>9</sub> O <sub>4</sub> P	-5.82	-5.81
0221tri	hexane	C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P	-6.78	-6.87
0222tri	hexane	C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> P	-7.24	-8.14
0425dbr	hexane	C <sub>7</sub> H <sub>3</sub> NOBr <sub>2</sub>	-9.67	-11.69
0506nit	hexane	CH <sub>3</sub> NO <sub>2</sub>	-2.90	-2.50
n008	hexane	C <sub>7</sub> H <sub>7</sub> NO	-7.77	-8.56
n011	hexane	C <sub>7</sub> H <sub>9</sub> N	-6.18	-6.52
0007nhe	heptane	C <sub>7</sub> H <sub>16</sub>	-4.65	-4.73
0035ben	heptane	C <sub>6</sub> H <sub>6</sub>	-4.00	-4.28
0036tol	heptane	C <sub>7</sub> H <sub>8</sub>	-4.78	-4.84
0038oxy	heptane	C <sub>8</sub> H <sub>10</sub>	-5.52	-5.40
0039mxy	heptane	C <sub>8</sub> H <sub>10</sub>	-5.67	-5.40
0040pxy	heptane	C <sub>8</sub> H <sub>10</sub>	-5.52	-5.40
0041nap	heptane	C <sub>10</sub> H <sub>8</sub>	-7.02	-6.90
0042ant	heptane	C <sub>14</sub> H <sub>10</sub>	-10.00	-9.77
0044met	heptane	CH <sub>4</sub> O	-1.29	-1.56
0045eth	heptane	C <sub>2</sub> H <sub>6</sub> O	-2.15	-2.42
0047pro	heptane	C <sub>3</sub> H <sub>8</sub> O	-3.01	-3.13
0049but	heptane	C <sub>4</sub> H <sub>10</sub> O	-3.66	-3.88
0052pen	heptane	C <sub>5</sub> H <sub>12</sub> O	-4.09	-4.53
0053phe	heptane	C <sub>6</sub> H <sub>6</sub> O	-5.32	-5.20
0054hex	heptane	C <sub>6</sub> H <sub>14</sub> O	-4.89	-5.27
0055ocr	heptane	C <sub>7</sub> H <sub>8</sub> O	-6.01	-5.91
0056mcr	heptane	C <sub>7</sub> H <sub>8</sub> O	-5.01	-5.88
0057pcr	heptane	C <sub>7</sub> H <sub>8</sub> O	-5.77	-5.89
0058hep	heptane	C <sub>7</sub> H <sub>16</sub> O	-5.60	-6.01
0068ani	heptane	C <sub>7</sub> H <sub>8</sub> O	-5.35	-5.33
0074ben	heptane	C <sub>7</sub> H <sub>6</sub> O	-5.50	-5.65
0075pro	heptane	C <sub>3</sub> H <sub>6</sub> O	-2.61	-2.77
0076but	heptane	C <sub>4</sub> H <sub>8</sub> O	-3.36	-3.60
0078pen	heptane	C <sub>5</sub> H <sub>10</sub> O	-4.07	-4.28
0080hex	heptane	C <sub>6</sub> H <sub>12</sub> O	-4.55	-4.96
0081dim	heptane	C <sub>6</sub> H <sub>12</sub> O	-4.30	-4.17
0082hep	heptane	C <sub>7</sub> H <sub>14</sub> O	-5.22	-5.64
0084met	heptane	C <sub>8</sub> H <sub>8</sub> O	-6.14	-6.23
0087pro	heptane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.06	-3.62
0088but	heptane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.05	-4.25
0089pen	heptane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-5.23	-4.91
0090hex	heptane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-6.54	-5.68
0093met	heptane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-2.97	-3.14
0094met	heptane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.63	-3.78
0095eth	heptane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.50	-3.67
0097pro	heptane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.09	-4.33
0098met	heptane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.92	-5.12
0099but	heptane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.83	-5.00
0100met	heptane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.63	-5.79
0101pen	heptane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.42	-5.67
0103eth	heptane	C <sub>2</sub> H <sub>7</sub> N	-2.09	-2.25
0106pro	heptane	C <sub>3</sub> H <sub>9</sub> N	-3.03	-2.97
0110but	heptane	C <sub>4</sub> H <sub>11</sub> N	-3.55	-3.71
0116pyr	heptane	C <sub>5</sub> H <sub>5</sub> N	-4.28	-4.66
0118ani	heptane	C <sub>6</sub> H <sub>7</sub> N	-5.38	-5.77
0126eth	heptane	C <sub>2</sub> H <sub>3</sub> N	-2.06	-2.45
0129ben	heptane	C <sub>7</sub> H <sub>5</sub> N	-5.33	-5.93
0134nit	heptane	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-6.14	-5.89
0157flu	heptane	C <sub>6</sub> H <sub>5</sub> F	-4.13	-4.25
0174chl	heptane	C <sub>6</sub> H <sub>5</sub> Cl	-5.15	-5.34
0175odi	heptane	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-6.01	-6.21
0176pdi	heptane	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-5.81	-6.38

0186bro	heptane	C <sub>6</sub> H <sub>5</sub> Br	-5.72	-5.66
0187dib	heptane	C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	-7.55	-7.11
0220tri	heptane	C <sub>3</sub> H <sub>9</sub> O <sub>4</sub> P	-5.59	-5.91
0221tri	heptane	C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P	-6.67	-6.96
0222tri	heptane	C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> P	-7.50	-8.23
0239oct	heptane	C <sub>8</sub> H <sub>16</sub> O	-5.68	-6.32
0245thi	heptane	C <sub>4</sub> H <sub>4</sub> S	-4.09	-4.13
0414dcl	heptane	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	-9.22	-10.29
0519dim	heptane	C <sub>4</sub> H <sub>9</sub> NO	-4.80	-5.11
n008	heptane	C <sub>7</sub> H <sub>7</sub> NO	-7.26	-8.43
n009	heptane	C <sub>7</sub> H <sub>9</sub> N	-6.28	-6.23
n010	heptane	C <sub>7</sub> H <sub>9</sub> N	-6.35	-6.41
n011	heptane	C <sub>7</sub> H <sub>9</sub> N	-6.15	-6.44
n186	heptane	C <sub>5</sub> H <sub>9</sub> NO	-5.80	-6.21
n200	heptane	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> F	-11.28	-9.04
n203	heptane	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> Br	-12.73	-9.67
test4001	heptane	C <sub>6</sub> H <sub>5</sub> I	-6.27	-6.27
0005npe	isooctane	C <sub>8</sub> H <sub>12</sub>	-3.21	-3.45
0006nhe	isooctane	C <sub>6</sub> H <sub>14</sub>	-3.08	-4.19
0008noc	isooctane	C <sub>8</sub> H <sub>18</sub>	-5.44	-5.60
0022pro	isooctane	C <sub>3</sub> H <sub>6</sub>	-1.61	-1.93
0025buta	isooctane	C <sub>4</sub> H <sub>8</sub>	-2.26	-2.71
0027pen	isooctane	C <sub>5</sub> H <sub>10</sub>	-2.36	-3.44
0035ben	isooctane	C <sub>6</sub> H <sub>6</sub>	-4.01	-4.36
0036tol	isooctane	C <sub>7</sub> H <sub>8</sub>	-4.68	-4.95
0039mxy	isooctane	C <sub>8</sub> H <sub>10</sub>	-5.12	-5.54
0045eth	isooctane	C <sub>7</sub> H <sub>6</sub> O	-2.44	-2.54
0047pro	isooctane	C <sub>3</sub> H <sub>8</sub> O	-3.00	-3.26
0049but	isooctane	C <sub>4</sub> H <sub>10</sub> O	-3.56	-4.00
0052pen	isooctane	C <sub>5</sub> H <sub>12</sub> O	-4.17	-4.64
0053phe	isooctane	C <sub>6</sub> H <sub>6</sub> O	-5.30	-5.43
0054hex	isooctane	C <sub>6</sub> H <sub>14</sub> O	-5.10	-5.38
0055ocr	isooctane	C <sub>7</sub> H <sub>8</sub> O	-5.68	-6.15
0057pcr	isooctane	C <sub>7</sub> H <sub>8</sub> O	-5.59	-6.14
0062dio	isooctane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.02	-4.53
0072but	isooctane	C <sub>4</sub> H <sub>8</sub> O	-3.45	-3.72
0073pen	isooctane	C <sub>5</sub> H <sub>10</sub> O	-4.24	-4.56
0075pro	isooctane	C <sub>3</sub> H <sub>8</sub> O	-2.44	-2.95
0076but	isooctane	C <sub>4</sub> H <sub>8</sub> O	-3.40	-3.75
0078pen	isooctane	C <sub>5</sub> H <sub>10</sub> O	-4.14	-4.43
0080hex	isooctane	C <sub>6</sub> H <sub>12</sub> O	-4.72	-5.12
0110but	isooctane	C <sub>4</sub> H <sub>11</sub> N	-3.57	-3.74
0118ani	isooctane	C <sub>6</sub> H <sub>7</sub> N	-5.20	-5.99
0131nit	isooctane	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-3.94	-4.19
0137ethb	isooctane	C <sub>2</sub> H <sub>6</sub> S	-3.13	-3.08
0138pro	isooctane	C <sub>3</sub> H <sub>8</sub> S	-3.78	-4.00
0162tri	isooctane	CHCl <sub>3</sub>	-3.06	-3.79
0240met	isooctane	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-6.71	-6.69
0506nit	isooctane	CH <sub>3</sub> NO <sub>2</sub>	-2.82	-2.68
0008noc	octane	C <sub>8</sub> H <sub>18</sub>	-5.28	-5.42
0036tol	octane	C <sub>7</sub> H <sub>8</sub>	-4.82	-4.84
0044met	octane	CH <sub>4</sub> O	-1.29	-1.41
0045eth	octane	C <sub>7</sub> H <sub>6</sub> O	-2.15	-2.31
0047pro	octane	C <sub>3</sub> H <sub>8</sub> O	-2.76	-3.10
0049but	octane	C <sub>4</sub> H <sub>10</sub> O	-3.69	-3.86
0052pen	octane	C <sub>5</sub> H <sub>12</sub> O	-4.10	-4.54
0053phe	octane	C <sub>6</sub> H <sub>6</sub> O	-5.47	-5.24
0054hex	octane	C <sub>6</sub> H <sub>14</sub> O	-4.86	-5.28
0055ocr	octane	C <sub>7</sub> H <sub>8</sub> O	-6.16	-5.97
0056mcr	octane	C <sub>7</sub> H <sub>8</sub> O	-5.19	-5.92
0057pcr	octane	C <sub>7</sub> H <sub>8</sub> O	-6.19	-5.93
0058hep	octane	C <sub>7</sub> H <sub>16</sub> O	-5.56	-6.02
0075pro	octane	C <sub>3</sub> H <sub>8</sub> O	-2.46	-2.75
0076but	octane	C <sub>4</sub> H <sub>8</sub> O	-3.24	-3.54
0078pen	octane	C <sub>5</sub> H <sub>10</sub> O	-3.97	-4.23
0080hex	octane	C <sub>6</sub> H <sub>12</sub> O	-4.60	-4.91
0081dim	octane	C <sub>6</sub> H <sub>12</sub> O	-4.21	-4.12
0082hep	octane	C <sub>7</sub> H <sub>14</sub> O	-5.25	-5.59
0093met	octane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.06	-3.06
0094met	octane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.57	-3.73
0095eth	octane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.48	-3.61
0097pro	octane	C <sub>3</sub> H <sub>10</sub> O <sub>2</sub>	-4.09	-4.27
0098met	octane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.86	-5.07
0099but	octane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.80	-4.94
0100met	octane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.53	-5.74
0101pen	octane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.36	-5.61
0103eth	octane	C <sub>2</sub> H <sub>7</sub> N	-2.04	-2.09
0106pro	octane	C <sub>3</sub> H <sub>9</sub> N	-3.00	-2.81
0110but	octane	C <sub>4</sub> H <sub>11</sub> N	-3.44	-3.55
0111die	octane	C <sub>4</sub> H <sub>11</sub> N	-3.42	-3.60
0117met	octane	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub>	-4.70	-5.76
0118ani	octane	C <sub>6</sub> H <sub>7</sub> N	-4.84	-5.64
0131nit	octane	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-3.95	-3.85

0230eth	octane	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub>	-5.51	-6.53
n009	octane	C <sub>7</sub> H <sub>9</sub> N	-6.06	-6.08
n010	octane	C <sub>7</sub> H <sub>9</sub> N	-6.15	-6.36
n011	octane	C <sub>7</sub> H <sub>9</sub> N	-6.00	-6.39
0044met	nonane	CH <sub>4</sub> O	-1.29	-1.27
0045eth	nonane	C <sub>2</sub> H <sub>6</sub> O	-2.15	-2.18
0047pro	nonane	C <sub>3</sub> H <sub>8</sub> O	-2.76	-3.02
0049but	nonane	C <sub>4</sub> H <sub>10</sub> O	-3.77	-3.85
0052pen	nonane	C <sub>5</sub> H <sub>12</sub> O	-3.92	-4.58
0053phe	nonane	C <sub>6</sub> H <sub>6</sub> O	-5.60	-5.29
0054hex	nonane	C <sub>6</sub> H <sub>14</sub> O	-4.97	-5.33
0055ocr	nonane	C <sub>7</sub> H <sub>8</sub> O	-6.20	-6.02
0058hep	nonane	C <sub>7</sub> H <sub>16</sub> O	-5.62	-6.07
0076but	nonane	C <sub>4</sub> H <sub>8</sub> O	-3.20	-3.48
0078pen	nonane	C <sub>5</sub> H <sub>10</sub> O	-3.97	-4.17
0080hex	nonane	C <sub>6</sub> H <sub>12</sub> O	-4.59	-4.85
0081dim	nonane	C <sub>6</sub> H <sub>12</sub> O	-4.19	-4.08
0082hep	nonane	C <sub>7</sub> H <sub>14</sub> O	-5.24	-5.53
0093met	nonane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.02	-2.87
0094met	nonane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.50	-3.60
0095eth	nonane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.45	-3.50
0097pro	nonane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.07	-4.21
0098met	nonane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.85	-5.01
0099but	nonane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.69	-4.88
0100met	nonane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.51	-5.68
0101pen	nonane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.33	-5.55
0103eth	nonane	C <sub>7</sub> H <sub>7</sub> N	-1.98	-1.94
0106pro	nonane	C <sub>3</sub> H <sub>9</sub> N	-2.96	-2.66
0110but	nonane	C <sub>4</sub> H <sub>11</sub> N	-3.55	-3.44
0511non	nonane	C <sub>6</sub> H <sub>20</sub>	-5.91	-6.09
0008noc	decane	C <sub>8</sub> H <sub>18</sub>	-5.18	-5.37
0035ben	decane	C <sub>6</sub> H <sub>6</sub>	-3.80	-3.96
0036tol	decane	C <sub>7</sub> H <sub>8</sub>	-4.65	-4.64
0037eth	decane	C <sub>8</sub> H <sub>10</sub>	-5.25	-5.40
0044met	decane	CH <sub>4</sub> O	-1.29	-1.21
0045eth	decane	C <sub>2</sub> H <sub>6</sub> O	-2.44	-2.12
0047pro	decane	C <sub>3</sub> H <sub>8</sub> O	-2.76	-2.97
0049but	decane	C <sub>4</sub> H <sub>10</sub> O	-3.77	-3.79
0052pen	decane	C <sub>5</sub> H <sub>12</sub> O	-3.92	-4.54
0053phe	decane	C <sub>6</sub> H <sub>6</sub> O	-5.50	-5.32
0054hex	decane	C <sub>6</sub> H <sub>14</sub> O	-4.97	-5.35
0057pcr	decane	C <sub>7</sub> H <sub>8</sub> O	-6.00	-6.03
0058hep	decane	C <sub>7</sub> H <sub>16</sub> O	-5.62	-6.11
0062dio	decane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.97	-4.16
0075pro	decane	C <sub>3</sub> H <sub>6</sub> O	-2.47	-2.54
0076but	decane	C <sub>4</sub> H <sub>8</sub> O	-3.30	-3.36
0078pen	decane	C <sub>5</sub> H <sub>10</sub> O	-3.93	-4.11
0080hex	decane	C <sub>6</sub> H <sub>12</sub> O	-4.61	-4.79
0081dim	decane	C <sub>6</sub> H <sub>12</sub> O	-4.15	-4.02
0082hep	decane	C <sub>7</sub> H <sub>14</sub> O	-5.18	-5.47
0093met	decane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-2.98	-2.70
0094met	decane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.49	-3.43
0095eth	decane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.43	-3.33
0097pro	decane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.02	-4.07
0098met	decane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.77	-4.93
0099but	decane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.66	-4.81
0100met	decane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.48	-5.62
0101pen	decane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.31	-5.49
0103eth	decane	C <sub>7</sub> H <sub>7</sub> N	-1.92	-1.81
0106pro	decane	C <sub>3</sub> H <sub>9</sub> N	-2.96	-2.59
0110but	decane	C <sub>4</sub> H <sub>11</sub> N	-3.55	-3.37
0157flu	decane	C <sub>6</sub> H <sub>5</sub> F	-3.48	-3.89
0173tri	decane	C <sub>3</sub> HCl <sub>3</sub>	-3.84	-3.95
0174chl	decane	C <sub>6</sub> H <sub>5</sub> Cl	-4.93	-5.29
0186bro	decane	C <sub>6</sub> H <sub>5</sub> Br	-5.43	-5.66
0233ethb	decane	C <sub>2</sub> H <sub>5</sub> NO	-2.85	-4.31
0506nit	decane	CH <sub>3</sub> NO <sub>2</sub>	-2.81	-2.29
0512dec	decane	C <sub>10</sub> H <sub>22</sub>	-6.53	-6.76
n011	decane	C <sub>7</sub> H <sub>9</sub> N	-6.05	-6.13
0035ben	undecane	C <sub>6</sub> H <sub>6</sub>	-4.05	-3.87
0036tol	undecane	C <sub>7</sub> H <sub>8</sub>	-4.81	-4.55
0037eth	undecane	C <sub>8</sub> H <sub>10</sub>	-5.44	-5.31
0110but	undecane	C <sub>4</sub> H <sub>11</sub> N	-3.55	-3.32
0162tri	undecane	CHCl <sub>3</sub>	-3.42	-3.40
0165tri	undecane	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	-3.82	-4.67
0172Edi	undecane	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	-3.60	-3.23
0173tri	undecane	C <sub>2</sub> HCl <sub>3</sub>	-3.87	-3.89
0174chl	undecane	C <sub>6</sub> H <sub>5</sub> Cl	-5.12	-5.20
0175odi	undecane	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-6.11	-6.25
0179tri	undecane	CHBr <sub>3</sub>	-4.84	-5.27
0204tet	undecane	C <sub>2</sub> Cl <sub>4</sub>	-4.63	-4.51
0520und	undecane	C <sub>12</sub> H <sub>26</sub>	-7.22	-8.11
0045eth	dodecane	C <sub>2</sub> H <sub>6</sub> O	-2.06	-2.02



0047pro	dodecane	C <sub>12</sub> H <sub>26</sub> O	-2.74	-2.86
0049but	dodecane	C <sub>12</sub> H <sub>24</sub> O	-3.47	-3.68
0052pen	dodecane	C <sub>12</sub> H <sub>22</sub> O	-4.09	-4.44
0054hex	dodecane	C <sub>12</sub> H <sub>20</sub> O	-4.28	-5.24
0058hep	dodecane	C <sub>12</sub> H <sub>18</sub> O	-5.41	-6.05
0084met	dodecane	C <sub>12</sub> H <sub>16</sub> O	-6.11	-5.94
0513dod	dodecane	C <sub>12</sub> H <sub>26</sub>	-7.83	-8.10
0003pro	cyclohexane	C <sub>6</sub> H <sub>12</sub> O	-2.09	-1.70
0004nbu	cyclohexane	C <sub>6</sub> H <sub>10</sub> O	-2.86	-2.51
0005npe	cyclohexane	C <sub>6</sub> H <sub>12</sub>	-3.50	-3.25
0008noc	cyclohexane	C <sub>6</sub> H <sub>18</sub>	-5.63	-5.42
0018cyc	cyclohexane	C <sub>6</sub> H <sub>12</sub>	-4.43	-4.19
0035ben	cyclohexane	C <sub>6</sub> H <sub>6</sub>	-4.19	-4.40
0036tol	cyclohexane	C <sub>7</sub> H <sub>8</sub>	-4.90	-5.03
0037eth	cyclohexane	C <sub>8</sub> H <sub>10</sub>	-4.97	-5.67
0038oxy	cyclohexane	C <sub>8</sub> H <sub>10</sub>	-5.54	-5.65
0039mxy	cyclohexane	C <sub>8</sub> H <sub>10</sub>	-5.52	-5.63
0041nap	cyclohexane	C <sub>10</sub> H <sub>8</sub>	-7.17	-7.38
0044met	cyclohexane	CH <sub>4</sub> O	-1.29	-1.74
0045eth	cyclohexane	C <sub>2</sub> H <sub>6</sub> O	-2.42	-2.65
0047pro	cyclohexane	C <sub>3</sub> H <sub>8</sub> O	-2.73	-3.43
0048pro	cyclohexane	C <sub>3</sub> H <sub>8</sub> O	-2.37	-3.18
0049but	cyclohexane	C <sub>4</sub> H <sub>10</sub> O	-3.52	-4.18
0050met	cyclohexane	C <sub>4</sub> H <sub>10</sub> O	-2.93	-3.89
0052pen	cyclohexane	C <sub>5</sub> H <sub>12</sub> O	-3.61	-4.85
0053phe	cyclohexane	C <sub>6</sub> H <sub>6</sub> O	-5.57	-5.62
0054hex	cyclohexane	C <sub>6</sub> H <sub>14</sub> O	-5.31	-5.59
0055ocr	cyclohexane	C <sub>7</sub> H <sub>8</sub> O	-6.02	-6.34
0056mcr	cyclohexane	C <sub>7</sub> H <sub>8</sub> O	-5.20	-6.32
0057pcr	cyclohexane	C <sub>7</sub> H <sub>8</sub> O	-5.89	-6.33
0058hep	cyclohexane	C <sub>7</sub> H <sub>16</sub> O	-6.02	-6.33
0062dio	cyclohexane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.17	-4.52
0063die	cyclohexane	C <sub>4</sub> H <sub>10</sub> O	-3.03	-3.37
0068ani	cyclohexane	C <sub>7</sub> H <sub>8</sub> O	-5.38	-5.66
0074ben	cyclohexane	C <sub>7</sub> H <sub>6</sub> O	-5.71	-5.98
0075pro	cyclohexane	C <sub>3</sub> H <sub>6</sub> O	-2.67	-3.01
0076but	cyclohexane	C <sub>4</sub> H <sub>8</sub> O	-3.48	-3.87
0078pen	cyclohexane	C <sub>5</sub> H <sub>10</sub> O	-4.19	-4.56
0079pen	cyclohexane	C <sub>5</sub> H <sub>10</sub> O	-4.30	-4.59
0080hex	cyclohexane	C <sub>6</sub> H <sub>12</sub> O	-4.77	-5.24
0081dim	cyclohexane	C <sub>6</sub> H <sub>12</sub> O	-4.42	-4.59
0082hep	cyclohexane	C <sub>7</sub> H <sub>14</sub> O	-5.47	-5.92
0084met	cyclohexane	C <sub>8</sub> H <sub>8</sub> O	-6.29	-6.75
0086eth	cyclohexane	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-1.73	-3.16
0087pro	cyclohexane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.78	-4.00
0093met	cyclohexane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.06	-3.58
0094met	cyclohexane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.71	-4.05
0095eth	cyclohexane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.56	-4.06
0097pro	cyclohexane	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	-4.36	-4.67
0098met	cyclohexane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.04	-5.37
0099but	cyclohexane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.94	-5.32
0100met	cyclohexane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.75	-6.04
0101pen	cyclohexane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.71	-5.96
0103eth	cyclohexane	C <sub>2</sub> H <sub>7</sub> N	-2.04	-2.41
0107tri	cyclohexane	C <sub>3</sub> H <sub>9</sub> N	-2.63	-3.02
0111die	cyclohexane	C <sub>4</sub> H <sub>11</sub> N	-3.61	-3.81
0116pyr	cyclohexane	C <sub>5</sub> H <sub>5</sub> N	-4.30	-4.78
0118ani	cyclohexane	C <sub>6</sub> H <sub>7</sub> N	-5.52	-6.12
0119met	cyclohexane	C <sub>6</sub> H <sub>7</sub> N	-5.05	-5.54
0120met	cyclohexane	C <sub>6</sub> H <sub>7</sub> N	-5.14	-5.55
0121met	cyclohexane	C <sub>6</sub> H <sub>7</sub> N	-5.23	-5.56
0122Nme	cyclohexane	C <sub>7</sub> H <sub>9</sub> N	-6.33	-6.36
0125dim	cyclohexane	C <sub>7</sub> H <sub>9</sub> N	-5.51	-6.18
0126eth	cyclohexane	C <sub>2</sub> H <sub>3</sub> N	-1.87	-3.05
0129ben	cyclohexane	C <sub>7</sub> H <sub>5</sub> N	-5.54	-6.43
0131nit	cyclohexane	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-4.06	-4.56
0134nit	cyclohexane	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-6.62	-6.52
0135met	cyclohexane	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	-6.71	-7.41
0138pro	cyclohexane	C <sub>3</sub> H <sub>8</sub> S	-3.12	-4.16
0144thi	cyclohexane	C <sub>7</sub> H <sub>8</sub> S	-5.66	-7.50
0150mhy	cyclohexane	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-6.88	-7.30
0151phy	cyclohexane	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-7.19	-7.35
0157flu	cyclohexane	C <sub>6</sub> H <sub>5</sub> F	-3.59	-4.35
0165tri	cyclohexane	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	-4.08	-5.01
0173tri	cyclohexane	C <sub>2</sub> HCl <sub>3</sub>	-4.29	-4.31
0174chl	cyclohexane	C <sub>6</sub> H <sub>5</sub> Cl	-5.10	-5.46
0176pdi	cyclohexane	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-5.89	-6.60
0186bro	cyclohexane	C <sub>6</sub> H <sub>5</sub> Br	-5.29	-5.74
0207tri	cyclohexane	C <sub>2</sub> H <sub>3</sub> OF <sub>3</sub>	-1.53	-2.19
0215pbr	cyclohexane	C <sub>6</sub> H <sub>5</sub> OBr	-7.14	-7.79
0217wat	cyclohexane	H <sub>2</sub> O	-0.39	-1.56
0220tri	cyclohexane	C <sub>3</sub> H <sub>9</sub> O <sub>4</sub> P	-5.67	-6.07
0221tri	cyclohexane	C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P	-7.60	-7.11

0222tri	cyclohexane	C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> P	-7.71	-8.38
0240met	cyclohexane	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-7.01	-7.00
0244tet	cyclohexane	C <sub>5</sub> H <sub>10</sub> O	-4.41	-4.75
0246eth	cyclohexane	C <sub>8</sub> H <sub>10</sub> O	-6.00	-6.29
0421dfl	cyclohexane	CF <sub>2</sub> Cl <sub>2</sub>	-1.81	-1.93
0422ftc	cyclohexane	CFCl <sub>3</sub>	-2.63	-3.20
0425dbr	cyclohexane	C <sub>7</sub> H <sub>3</sub> NOBr <sub>2</sub>	-6.83	-12.26
0506nit	cyclohexane	CH <sub>3</sub> NO <sub>2</sub>	-2.86	-3.24
0515dim	cyclohexane	C <sub>3</sub> H <sub>7</sub> NO	-3.82	-4.97
0579pyy	cyclohexane	C <sub>4</sub> H <sub>5</sub> N	-3.77	-4.84
0582qui	cyclohexane	C <sub>6</sub> H <sub>7</sub> N	-7.38	-8.21
n008	cyclohexane	C <sub>7</sub> H <sub>7</sub> NO	-8.72	-9.12
n009	cyclohexane	C <sub>7</sub> H <sub>9</sub> N	-6.44	-6.59
n010	cyclohexane	C <sub>7</sub> H <sub>9</sub> N	-6.47	-6.77
n011	cyclohexane	C <sub>7</sub> H <sub>9</sub> N	-6.30	-6.79
test4001	cyclohexane	C <sub>6</sub> H <sub>5</sub> I	-6.26	-6.49
0075pro	perfluorobenzene	C <sub>3</sub> H <sub>6</sub> O	-3.82	-2.86
0078pen	perfluorobenzene	C <sub>3</sub> H <sub>10</sub> O	-5.10	-3.96
0080hex	perfluorobenzene	C <sub>6</sub> H <sub>12</sub> O	-5.55	-4.55
0081dim	perfluorobenzene	C <sub>6</sub> H <sub>12</sub> O	-5.26	-4.49
0082hep	perfluorobenzene	C <sub>7</sub> H <sub>14</sub> O	-6.15	-5.14
0093met	perfluorobenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.23	-3.34
0095eth	perfluorobenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.56	-3.85
0097pro	perfluorobenzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-5.06	-4.44
0098met	perfluorobenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.59	-4.94
0099but	perfluorobenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.52	-4.99
0100met	perfluorobenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.21	-5.50
0101pen	perfluorobenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.16	-5.55
0110but	perfluorobenzene	C <sub>4</sub> H <sub>11</sub> N	-4.13	-2.93
0505per	perfluorobenzene	C <sub>6</sub> F <sub>6</sub>	-4.42	-2.26
0506nit	perfluorobenzene	CH <sub>3</sub> NO <sub>2</sub>	-4.30	-3.18
0093met	pentadecane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-2.82	-2.47
0094met	pentadecane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.35	-3.10
0095eth	pentadecane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.37	-3.04
0097pro	pentadecane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-3.91	-3.71
0098met	pentadecane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.59	-4.56
0099but	pentadecane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.49	-4.46
0100met	pentadecane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.35	-5.30
0101pen	pentadecane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.18	-5.20
0516pen	pentadecane	C <sub>15</sub> H <sub>32</sub>	-9.91	-10.08
0001met	hexadecane	CH <sub>4</sub>	0.45	0.03
0002eth	hexadecane	C <sub>2</sub> H <sub>6</sub>	-0.67	-0.75
0003pro	hexadecane	C <sub>3</sub> H <sub>8</sub>	-1.43	-1.43
0004nbu	hexadecane	C <sub>4</sub> H <sub>10</sub>	-2.20	-2.09
0005npe	hexadecane	C <sub>5</sub> H <sub>12</sub>	-2.95	-2.86
0006nhe	hexadecane	C <sub>6</sub> H <sub>14</sub>	-3.64	-3.62
0007nhe	hexadecane	C <sub>7</sub> H <sub>16</sub>	-4.33	-4.37
0008noc	hexadecane	C <sub>8</sub> H <sub>18</sub>	-5.02	-5.13
0009nhe	hexadecane	C <sub>16</sub> H <sub>34</sub>	-10.52	-10.62
0010met	hexadecane	C <sub>4</sub> H <sub>10</sub>	-1.92	-1.99
0011dim	hexadecane	C <sub>5</sub> H <sub>12</sub>	-2.48	-2.27
0012met	hexadecane	C <sub>6</sub> H <sub>14</sub>	-3.48	-3.47
0013dim	hexadecane	C <sub>7</sub> H <sub>16</sub>	-3.87	-4.09
0014tri	hexadecane	C <sub>8</sub> H <sub>18</sub>	-4.24	-4.30
0016cyc	hexadecane	C <sub>3</sub> H <sub>6</sub>	-1.78	-2.43
0017cyc	hexadecane	C <sub>5</sub> H <sub>10</sub>	-3.38	-3.42
0018cyc	hexadecane	C <sub>6</sub> H <sub>12</sub>	-4.04	-4.21
0019met	hexadecane	C <sub>7</sub> H <sub>14</sub>	-4.43	-4.89
0021eth	hexadecane	C <sub>2</sub> H <sub>4</sub>	-0.39	-0.65
0022pro	hexadecane	C <sub>3</sub> H <sub>6</sub>	-1.29	-1.30
0023str	hexadecane	C <sub>4</sub> H <sub>6</sub>	-2.10	-1.95
0025buta	hexadecane	C <sub>4</sub> H <sub>8</sub>	-2.03	-1.98
0027pen	hexadecane	C <sub>5</sub> H <sub>10</sub>	-2.79	-2.75
0029hex	hexadecane	C <sub>6</sub> H <sub>12</sub>	-3.51	-3.55
0030eth	hexadecane	C <sub>2</sub> H <sub>2</sub>	-0.20	-0.69
0031pro	hexadecane	C <sub>3</sub> H <sub>4</sub>	-1.40	-1.32
0032but	hexadecane	C <sub>4</sub> H <sub>6</sub>	-2.07	-1.98
0033pen	hexadecane	C <sub>5</sub> H <sub>8</sub>	-2.74	-2.69
0034hex	hexadecane	C <sub>6</sub> H <sub>10</sub>	-3.42	-3.42
0035ben	hexadecane	C <sub>6</sub> H <sub>6</sub>	-3.80	-3.65
0036tol	hexadecane	C <sub>7</sub> H <sub>8</sub>	-4.54	-4.36
0037eth	hexadecane	C <sub>8</sub> H <sub>10</sub>	-5.15	-5.14
0038oxy	hexadecane	C <sub>8</sub> H <sub>10</sub>	-5.37	-5.02
0039mxy	hexadecane	C <sub>8</sub> H <sub>10</sub>	-5.24	-5.06
0040pxy	hexadecane	C <sub>8</sub> H <sub>10</sub>	-5.24	-5.06
0041nap	hexadecane	C <sub>10</sub> H <sub>8</sub>	-7.29	-6.69
0042ant	hexadecane	C <sub>14</sub> H <sub>10</sub>	-10.32	-9.61
0043chr	hexadecane	C <sub>18</sub> H <sub>12</sub>	-14.10	-12.49
0044met	hexadecane	CH <sub>4</sub> O	-1.32	-1.33
0045eth	hexadecane	C <sub>2</sub> H <sub>6</sub> O	-2.03	-2.13
0046eth	hexadecane	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	-2.81	-3.18
0047pro	hexadecane	C <sub>3</sub> H <sub>8</sub> O	-2.77	-2.91
0048pro	hexadecane	C <sub>3</sub> H <sub>8</sub> O	-2.47	-2.66

0049but	hexadecane	C <sub>4</sub> H <sub>10</sub> O	-3.55	-3.73
0050met	hexadecane	C <sub>4</sub> H <sub>10</sub> O	-2.74	-3.21
0051cyc	hexadecane	C <sub>5</sub> H <sub>10</sub> O	-4.42	-5.07
0052pen	hexadecane	C <sub>5</sub> H <sub>12</sub> O	-4.24	-4.47
0053phe	hexadecane	C <sub>6</sub> H <sub>6</sub> O	-5.14	-5.37
0054hex	hexadecane	C <sub>6</sub> H <sub>14</sub> O	-4.92	-5.27
0055ocr	hexadecane	C <sub>7</sub> H <sub>8</sub> O	-5.78	-6.16
0056mcr	hexadecane	C <sub>7</sub> H <sub>8</sub> O	-5.91	-6.17
0057per	hexadecane	C <sub>7</sub> H <sub>8</sub> O	-5.88	-6.19
0058hep	hexadecane	C <sub>7</sub> H <sub>16</sub> O	-5.62	-6.08
0059dec	hexadecane	C <sub>10</sub> H <sub>22</sub> O	-7.68	-8.45
0060dim	hexadecane	C <sub>2</sub> H <sub>6</sub> O	-1.49	-1.67
0061tet	hexadecane	C <sub>4</sub> H <sub>8</sub> O	-3.60	-3.72
0062dio	hexadecane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.82	-4.33
0063die	hexadecane	C <sub>4</sub> H <sub>10</sub> O	-2.81	-2.86
0066dim	hexadecane	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	-3.63	-3.79
0068ani	hexadecane	C <sub>7</sub> H <sub>8</sub> O	-5.35	-5.18
0069met	hexadecane	CH <sub>2</sub> O	-0.99	-0.95
0070eth	hexadecane	C <sub>2</sub> H <sub>4</sub> O	-1.68	-1.65
0071proa	hexadecane	C <sub>3</sub> H <sub>6</sub> O	-2.48	-2.41
0072but	hexadecane	C <sub>4</sub> H <sub>8</sub> O	-3.10	-3.17
0073pen	hexadecane	C <sub>5</sub> H <sub>10</sub> O	-3.89	-3.92
0074ben	hexadecane	C <sub>7</sub> H <sub>6</sub> O	-5.44	-5.31
0075pro	hexadecane	C <sub>3</sub> H <sub>6</sub> O	-2.31	-2.27
0076but	hexadecane	C <sub>4</sub> H <sub>8</sub> O	-3.12	-3.07
0077cyc	hexadecane	C <sub>5</sub> H <sub>8</sub> O	-4.39	-4.46
0078pen	hexadecane	C <sub>5</sub> H <sub>10</sub> O	-3.76	-3.80
0079pen	hexadecane	C <sub>5</sub> H <sub>10</sub> O	-3.83	-3.84
0080hex	hexadecane	C <sub>6</sub> H <sub>12</sub> O	-4.45	-4.54
0081dim	hexadecane	C <sub>6</sub> H <sub>12</sub> O	-3.94	-3.95
0082hep	hexadecane	C <sub>7</sub> H <sub>14</sub> O	-5.13	-5.28
0083hep	hexadecane	C <sub>7</sub> H <sub>14</sub> O	-5.20	-5.27
0084met	hexadecane	C <sub>8</sub> H <sub>8</sub> O	-6.14	-5.99
0085non	hexadecane	C <sub>9</sub> H <sub>18</sub> O	-6.46	-6.72
0086eth	hexadecane	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-2.39	-2.88
0087pro	hexadecane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.12	-3.74
0088but	hexadecane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.86	-4.45
0089pen	hexadecane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.61	-5.15
0090hex	hexadecane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.35	-5.94
0091met	hexadecane	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-1.99	-2.02
0092ethb	hexadecane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-2.59	-2.59
0093met	hexadecane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-2.67	-2.59
0094met	hexadecane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-2.68	-3.23
0095eth	hexadecane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.25	-3.18
0096met	hexadecane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.01	-3.98
0097pro	hexadecane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-3.93	-3.88
0098met	hexadecane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.69	-4.73
0099but	hexadecane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.61	-4.62
0100met	hexadecane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.43	-5.46
0101pen	hexadecane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.20	-5.36
0102eth	hexadecane	C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>	-13.69	-13.10
0103eth	hexadecane	C <sub>2</sub> H <sub>7</sub> N	-2.29	-1.83
0104dim	hexadecane	C <sub>2</sub> H <sub>7</sub> N	-2.18	-2.37
0106pro	hexadecane	C <sub>3</sub> H <sub>9</sub> N	-2.92	-2.53
0107tri	hexadecane	C <sub>3</sub> H <sub>9</sub> N	-2.21	-2.51
0111die	hexadecane	C <sub>4</sub> H <sub>11</sub> N	-3.27	-3.54
0113pen	hexadecane	C <sub>5</sub> H <sub>13</sub> N	-4.28	-4.10
0115dip	hexadecane	C <sub>6</sub> H <sub>15</sub> N	-4.57	-4.90
0116pyr	hexadecane	C <sub>5</sub> H <sub>5</sub> N	-4.10	-4.38
0118ani	hexadecane	C <sub>6</sub> H <sub>7</sub> N	-5.44	-5.42
0119met	hexadecane	C <sub>6</sub> H <sub>7</sub> N	-4.68	-5.12
0120met	hexadecane	C <sub>6</sub> H <sub>7</sub> N	-4.91	-5.17
0121met	hexadecane	C <sub>6</sub> H <sub>7</sub> N	-4.89	-5.14
0122Nme	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-6.19	-6.03
0123dim	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-5.52	-5.83
0124dim	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-5.52	-5.85
0125dim	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-5.27	-5.77
0126eth	hexadecane	C <sub>2</sub> H <sub>5</sub> N	-2.37	-2.26
0127pro	hexadecane	C <sub>3</sub> H <sub>5</sub> N	-2.84	-2.98
0128butb	hexadecane	C <sub>4</sub> H <sub>7</sub> N	-3.48	-3.64
0129ben	hexadecane	C <sub>7</sub> H <sub>5</sub> N	-5.51	-5.52
0130nit	hexadecane	C <sub>7</sub> H <sub>5</sub> NO <sub>2</sub>	-3.29	-3.12
0131nit	hexadecane	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-3.95	-3.66
0132nit	hexadecane	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-3.47	-3.66
0133nit	hexadecane	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	-4.66	-4.37
0134nit	hexadecane	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-6.22	-5.57
0135met	hexadecane	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	-6.52	-6.27
0137ethb	hexadecane	C <sub>2</sub> H <sub>6</sub> S	-2.96	-2.82
0138pro	hexadecane	C <sub>3</sub> H <sub>8</sub> S	-3.66	-3.60
0139thi	hexadecane	C <sub>6</sub> H <sub>6</sub> S	-5.61	-6.03
0140dim	hexadecane	C <sub>2</sub> H <sub>6</sub> S	-3.05	-2.38
0141dim	hexadecane	C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>	-4.84	-4.68
0142die	hexadecane	C <sub>4</sub> H <sub>10</sub> S	-4.23	-4.08

0143dip	hexadecane	C <sub>6</sub> H <sub>14</sub> S	-5.61	-5.57
0145pro	hexadecane	C <sub>3</sub> H <sub>6</sub> O	-2.73	-2.69
0155flu	hexadecane	C <sub>2</sub> H <sub>5</sub> F	-0.76	-1.00
0157flu	hexadecane	C <sub>6</sub> H <sub>5</sub> F	-4.03	-3.63
0158flu	hexadecane	C <sub>6</sub> H <sub>13</sub> F	-4.03	-3.76
0159flu	hexadecane	C <sub>8</sub> H <sub>17</sub> F	-5.25	-5.26
0161dic	hexadecane	CH <sub>2</sub> Cl <sub>2</sub>	-2.76	-2.87
0162tri	hexadecane	CHCl <sub>3</sub>	-3.38	-3.52
0163chl	hexadecane	C <sub>2</sub> H <sub>5</sub> Cl	-2.29	-2.36
0165tri	hexadecane	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	-3.73	-4.76
0166tri	hexadecane	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	-4.49	-5.18
0167chla	hexadecane	C <sub>3</sub> H <sub>7</sub> Cl	-2.86	-3.01
0168chl	hexadecane	C <sub>3</sub> H <sub>7</sub> Cl	-2.69	-2.97
0170chl	hexadecane	C <sub>3</sub> H <sub>5</sub> Cl	-2.88	-2.99
0171Zdi	hexadecane	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	-3.33	-2.96
0172Edi	hexadecane	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	-3.11	-3.28
0173tri	hexadecane	C <sub>2</sub> HCl <sub>3</sub>	-4.08	-3.78
0174chl	hexadecane	C <sub>6</sub> H <sub>5</sub> Cl	-4.99	-5.03
0175odi	hexadecane	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-6.16	-6.15
0176pdi	hexadecane	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-6.02	-6.36
0178dib	hexadecane	CH <sub>2</sub> Br <sub>2</sub>	-3.94	-4.27
0179tri	hexadecane	CHBr <sub>3</sub>	-5.16	-5.16
0180bro	hexadecane	C <sub>2</sub> H <sub>5</sub> Br	-2.89	-2.93
0182bro	hexadecane	C <sub>3</sub> H <sub>7</sub> Br	-3.57	-3.61
0183bro	hexadecane	C <sub>3</sub> H <sub>7</sub> Br	-3.26	-3.55
0184bro	hexadecane	C <sub>4</sub> H <sub>9</sub> Br	-4.24	-4.27
0185bro	hexadecane	C <sub>5</sub> H <sub>11</sub> Br	-4.93	-4.91
0186bro	hexadecane	C <sub>6</sub> H <sub>5</sub> Br	-5.51	-5.55
0201bro	hexadecane	C <sub>2</sub> HF <sub>3</sub> ClBr	-2.97	-3.23
0203bro	hexadecane	C <sub>2</sub> HF <sub>4</sub> Br	-1.87	-1.92
0204tet	hexadecane	C <sub>2</sub> Cl <sub>4</sub>	-4.88	-4.44
0206tri	hexadecane	C <sub>2</sub> F <sub>3</sub> Cl <sub>3</sub>	-2.89	-3.55
0207tri	hexadecane	C <sub>2</sub> H <sub>3</sub> OF <sub>3</sub>	-1.67	-1.68
0210dic	hexadecane	C <sub>3</sub> H <sub>4</sub> OF <sub>2</sub> Cl <sub>2</sub>	-3.90	-4.03
0214tri	hexadecane	C <sub>4</sub> H <sub>5</sub> OF <sub>3</sub>	-1.91	-2.13
0216amm	hexadecane	H <sub>3</sub> N	-0.93	-0.26
0217wat	hexadecane	H <sub>2</sub> O	-0.35	-1.42
0219hyd	hexadecane	H <sub>2</sub> S	-0.72	-1.76
0223die	hexadecane	C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>	-5.74	-5.93
0233ethb	hexadecane	C <sub>2</sub> H <sub>5</sub> NO	-3.33	-4.20
0236oct	hexadecane	C <sub>8</sub> H <sub>18</sub> O	-6.30	-6.87
0237oct	hexadecane	C <sub>8</sub> H <sub>16</sub> O	-5.98	-6.17
0239oct	hexadecane	C <sub>8</sub> H <sub>16</sub> O	-5.81	-6.02
0240met	hexadecane	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-6.31	-6.29
0242dii	hexadecane	C <sub>6</sub> H <sub>14</sub> O	-4.02	-3.91
0244tet	hexadecane	C <sub>5</sub> H <sub>10</sub> O	-4.08	-4.45
0245thi	hexadecane	C <sub>4</sub> H <sub>4</sub> S	-4.01	-4.02
0246eth	hexadecane	C <sub>8</sub> H <sub>10</sub> O	-5.64	-5.89
0400hyd	hexadecane	H <sub>2</sub>	1.64	1.40
0417brp	hexadecane	C <sub>3</sub> H <sub>5</sub> Br	-3.42	-3.59
0418bri	hexadecane	C <sub>4</sub> H <sub>9</sub> Br	-4.04	-4.17
0419brt	hexadecane	C <sub>7</sub> H <sub>7</sub> Br	-6.36	-6.37
0420pbr	hexadecane	C <sub>7</sub> H <sub>7</sub> Br	-6.19	-6.26
0423brt	hexadecane	CCl <sub>3</sub> Br	-4.46	-4.99
0431pho	hexadecane	C <sub>3</sub> H <sub>9</sub> O <sub>3</sub> P	-5.43	-4.93
0471dim	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-2.58	-5.85
0506nit	hexadecane	CH <sub>3</sub> NO <sub>2</sub>	-2.58	-2.57
0571dim	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-2.52	-5.91
0574eth	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-2.45	-5.92
0939tet	hexadecane	C <sub>4</sub> H <sub>12</sub> Si	-2.92	-2.42
n007	hexadecane	CH <sub>4</sub> N <sub>2</sub> O	-6.37	-3.83
n009	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-6.08	-5.95
n011	hexadecane	C <sub>7</sub> H <sub>9</sub> N	-6.04	-6.15
n127	hexadecane	CH <sub>3</sub> NO	-2.91	-3.30
test4001	hexadecane	C <sub>6</sub> H <sub>5</sub> I	-6.25	-6.28
test4002	hexadecane	CH <sub>2</sub> I <sub>2</sub>	-5.26	-5.57
test4003	hexadecane	CH <sub>3</sub> I	-2.88	-2.93
test4004	hexadecane	C <sub>2</sub> H <sub>5</sub> I	-3.51	-3.60
test4005	hexadecane	C <sub>3</sub> H <sub>5</sub> I	-4.10	-4.04
test4006	hexadecane	C <sub>3</sub> H <sub>7</sub> I	-4.27	-4.28
test4007	hexadecane	C <sub>4</sub> H <sub>9</sub> I	-4.95	-5.01
test4008	hexadecane	C <sub>5</sub> H <sub>11</sub> I	-5.63	-5.76
0036tol	decalin	C <sub>7</sub> H <sub>8</sub>	-4.37	-4.63
0053pce	decalin	C <sub>6</sub> H <sub>6</sub> O	-5.38	-5.83
0056mcr	decalin	C <sub>7</sub> H <sub>8</sub> O	-5.11	-6.61
0057pcr	decalin	C <sub>7</sub> H <sub>8</sub> O	-5.68	-6.62
0068ani	decalin	C <sub>7</sub> H <sub>8</sub> O	-5.00	-5.38
0084met	decalin	C <sub>8</sub> H <sub>8</sub> O	-6.23	-6.55
0086eth	decalin	C <sub>7</sub> H <sub>4</sub> O <sub>2</sub>	-4.49	-3.51
0087pro	decalin	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.42	-4.23
0093met	decalin	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-2.90	-3.05
0094met	decalin	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.50	-3.44
0095eth	decalin	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.47	-3.47

0097pro	decalin	C <sub>7</sub> H <sub>10</sub> O <sub>2</sub>	-4.05	-4.18
0098met	decalin	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.83	-4.92
0099but	decalin	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-4.71	-4.91
0100met	decalin	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.51	-5.66
0101pen	decalin	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.44	-5.64
0110but	decalin	C <sub>4</sub> H <sub>11</sub> N	-3.72	-3.75
0118ani	decalin	C <sub>6</sub> H <sub>7</sub> N	-5.78	-5.88
0122Nme	decalin	C <sub>7</sub> H <sub>9</sub> N	-6.41	-6.27
0129ben	decalin	C <sub>7</sub> H <sub>5</sub> N	-5.86	-5.92
0134nit	decalin	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-6.36	-6.44
0144thi	decalin	C <sub>7</sub> H <sub>5</sub> S	-5.54	-7.18
0157flu	decalin	C <sub>6</sub> H <sub>5</sub> F	-3.44	-3.83
0174chl	decalin	C <sub>6</sub> H <sub>5</sub> Cl	-4.61	-5.24
0186bro	decalin	C <sub>6</sub> H <sub>5</sub> Br	-5.25	-5.59
0240met	decalin	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-6.76	-6.74
test4001	decalin	C <sub>6</sub> H <sub>5</sub> I	-5.96	-6.36
0008noc	carbon tetrachloride	C <sub>8</sub> H <sub>18</sub>	-5.39	-5.42
0024met	carbon tetrachloride	C <sub>4</sub> H <sub>8</sub>	-2.63	-2.35
0025buta	carbon tetrachloride	C <sub>4</sub> H <sub>8</sub>	-2.48	-2.44
0028Epe	carbon tetrachloride	C <sub>5</sub> H <sub>10</sub>	-3.46	-3.25
0035ben	carbon tetrachloride	C <sub>6</sub> H <sub>6</sub>	-4.50	-4.41
0036tol	carbon tetrachloride	C <sub>7</sub> H <sub>8</sub>	-5.12	-5.10
0037eth	carbon tetrachloride	C <sub>6</sub> H <sub>10</sub>	-5.67	-5.75
0038oxy	carbon tetrachloride	C <sub>8</sub> H <sub>10</sub>	-6.07	-5.72
0039mxy	carbon tetrachloride	C <sub>8</sub> H <sub>10</sub>	-5.71	-5.71
0041nap	carbon tetrachloride	C <sub>10</sub> H <sub>8</sub>	-7.55	-7.48
0044met	carbon tetrachloride	CH <sub>4</sub> O	-2.25	-1.88
0045eth	carbon tetrachloride	C <sub>2</sub> H <sub>6</sub> O	-2.96	-2.78
0047pro	carbon tetrachloride	C <sub>3</sub> H <sub>8</sub> O	-3.64	-3.61
0048pro	carbon tetrachloride	C <sub>3</sub> H <sub>8</sub> O	-3.15	-3.34
0049but	carbon tetrachloride	C <sub>4</sub> H <sub>10</sub> O	-4.20	-4.36
0050met	carbon tetrachloride	C <sub>4</sub> H <sub>10</sub> O	-3.40	-4.01
0052pen	carbon tetrachloride	C <sub>5</sub> H <sub>12</sub> O	-4.73	-5.02
0053phe	carbon tetrachloride	C <sub>6</sub> H <sub>6</sub> O	-6.14	-5.80
0054hex	carbon tetrachloride	C <sub>6</sub> H <sub>14</sub> O	-5.04	-5.75
0055ocr	carbon tetrachloride	C <sub>7</sub> H <sub>8</sub> O	-6.51	-6.52
0057pcr	carbon tetrachloride	C <sub>7</sub> H <sub>8</sub> O	-6.32	-6.47
0058hep	carbon tetrachloride	C <sub>7</sub> H <sub>16</sub> O	-6.49	-6.49
0062dio	carbon tetrachloride	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.97	-4.67
0068ani	carbon tetrachloride	C <sub>7</sub> H <sub>8</sub> O	-5.49	-5.76
0074ben	carbon tetrachloride	C <sub>7</sub> H <sub>6</sub> O	-6.11	-6.24
0075pro	carbon tetrachloride	C <sub>3</sub> H <sub>6</sub> O	-3.35	-3.23
0076but	carbon tetrachloride	C <sub>4</sub> H <sub>8</sub> O	-4.09	-4.05
0077cyc	carbon tetrachloride	C <sub>5</sub> H <sub>8</sub> O	-5.26	-5.04
0078pen	carbon tetrachloride	C <sub>5</sub> H <sub>10</sub> O	-4.81	-4.74
0080hex	carbon tetrachloride	C <sub>6</sub> H <sub>12</sub> O	-5.47	-5.42
0082hep	carbon tetrachloride	C <sub>7</sub> H <sub>14</sub> O	-6.12	-6.11
0084met	carbon tetrachloride	C <sub>8</sub> H <sub>8</sub> O	-7.10	-6.97
0086eth	carbon tetrachloride	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-3.64	-3.41
0087pro	carbon tetrachloride	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.09	-4.25
0088but	carbon tetrachloride	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.81	-4.92
0090hex	carbon tetrachloride	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-6.99	-6.33
0093met	carbon tetrachloride	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.82	-3.72
0094met	carbon tetrachloride	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.43	-4.25
0095eth	carbon tetrachloride	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.40	-4.25
0097pro	carbon tetrachloride	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-5.03	-4.88
0098met	carbon tetrachloride	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.71	-5.58
0099but	carbon tetrachloride	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.59	-5.53
0100met	carbon tetrachloride	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.39	-6.25
0101pen	carbon tetrachloride	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.35	-6.18
0103eth	carbon tetrachloride	C <sub>2</sub> H <sub>7</sub> N	-2.77	-2.55
0104dim	carbon tetrachloride	C <sub>2</sub> H <sub>7</sub> N	-2.75	-2.83
0106pro	carbon tetrachloride	C <sub>3</sub> H <sub>9</sub> N	-3.59	-3.25
0107tri	carbon tetrachloride	C <sub>3</sub> H <sub>9</sub> N	-3.09	-3.06
0110but	carbon tetrachloride	C <sub>4</sub> H <sub>11</sub> N	-5.35	-3.97
0111die	carbon tetrachloride	C <sub>4</sub> H <sub>11</sub> N	-4.12	-3.89
0116pyr	carbon tetrachloride	C <sub>5</sub> H <sub>5</sub> N	-5.01	-4.92
0118ani	carbon tetrachloride	C <sub>6</sub> H <sub>7</sub> N	-6.10	-6.31
0122Nme	carbon tetrachloride	C <sub>7</sub> H <sub>9</sub> N	-6.58	-6.57
0129ben	carbon tetrachloride	C <sub>7</sub> H <sub>5</sub> N	-6.28	-6.66
0131nit	carbon tetrachloride	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-4.49	-4.67
0134nit	carbon tetrachloride	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-6.92	-6.58
0135met	carbon tetrachloride	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	-7.49	-7.44
0144thi	carbon tetrachloride	C <sub>7</sub> H <sub>5</sub> S	-5.66	-7.75
0151phy	carbon tetrachloride	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-8.16	-7.57
0157flu	carbon tetrachloride	C <sub>6</sub> H <sub>5</sub> F	-3.64	-4.47
0174chl	carbon tetrachloride	C <sub>6</sub> H <sub>5</sub> Cl	-5.21	-5.51
0176pdi	carbon tetrachloride	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-6.28	-6.67
0186bro	carbon tetrachloride	C <sub>6</sub> H <sub>5</sub> Br	-5.85	-5.84
0215pbr	carbon tetrachloride	C <sub>6</sub> H <sub>5</sub> OBr	-7.86	-7.88
0216amm	carbon tetrachloride	H <sub>3</sub> N	-1.06	-1.13
0217wat	carbon tetrachloride	H <sub>2</sub> O	-0.85	-1.74
0220tri	carbon tetrachloride	C <sub>3</sub> H <sub>9</sub> O <sub>4</sub> P	-7.24	-6.50

0221tri	carbon tetrachloride	C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P	-7.51	-7.62
0222tri	carbon tetrachloride	C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> P	-8.60	-8.88
0228met	carbon tetrachloride	CH <sub>3</sub> N	-2.53	-2.08
0240met	carbon tetrachloride	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-7.19	-7.20
0506nit	carbon tetrachloride	CH <sub>3</sub> NO <sub>2</sub>	-3.52	-3.29
0525car	carbon tetrachloride	CCl <sub>4</sub>	-4.35	-4.43
n008	carbon tetrachloride	C <sub>7</sub> H <sub>7</sub> NO	-9.13	-9.51
n009	carbon tetrachloride	C <sub>7</sub> H <sub>9</sub> N	-7.16	-6.83
n010	carbon tetrachloride	C <sub>7</sub> H <sub>9</sub> N	-7.23	-6.97
n011	carbon tetrachloride	C <sub>7</sub> H <sub>9</sub> N	-7.24	-6.98
test4001	carbon tetrachloride	C <sub>6</sub> H <sub>5</sub> I	-6.50	-6.67
0093met	isopropyltoluene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.32	-3.32
0094met	isopropyltoluene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.14	-3.69
0098met	isopropyltoluene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.33	-5.12
0100met	isopropyltoluene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.06	-5.83
0101pen	isopropyltoluene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.02	-5.84
0110but	isopropyltoluene	C <sub>4</sub> H <sub>11</sub> N	-4.22	-3.78
0053phe	mesitylene	C <sub>8</sub> H <sub>6</sub> O	-6.80	-6.10
0076but	mesitylene	C <sub>4</sub> H <sub>8</sub> O	-3.95	-3.64
0078pen	mesitylene	C <sub>5</sub> H <sub>10</sub> O	-4.80	-4.39
0080hex	mesitylene	C <sub>6</sub> H <sub>12</sub> O	-5.34	-5.15
0081dim	mesitylene	C <sub>6</sub> H <sub>12</sub> O	-4.77	-4.40
0082hep	mesitylene	C <sub>7</sub> H <sub>14</sub> O	-5.99	-5.90
0531mes	mesitylene	C <sub>9</sub> H <sub>12</sub>	-6.40	-6.29
0053phe	tetrachloroethene	C <sub>6</sub> H <sub>6</sub> O	-6.10	-6.16
0075pro	tetrachloroethene	C <sub>3</sub> H <sub>6</sub> O	-3.09	-3.34
0093met	tetrachloroethene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.63	-3.65
0094met	tetrachloroethene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.39	-4.17
0095eth	tetrachloroethene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.22	-4.20
0097pro	tetrachloroethene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.80	-4.90
0098met	tetrachloroethene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.41	-5.64
0099but	tetrachloroethene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.35	-5.63
0110but	tetrachloroethene	C <sub>4</sub> H <sub>11</sub> N	-4.49	-3.95
0204tet	tetrachloroethene	C <sub>2</sub> Cl <sub>4</sub>	-5.39	-4.79
0005npe	benzene	C <sub>5</sub> H <sub>12</sub>	-2.99	-3.26
0006nhe	benzene	C <sub>6</sub> H <sub>14</sub>	-3.62	-4.00
0008noc	benzene	C <sub>8</sub> H <sub>18</sub>	-5.35	-5.48
0018cyc	benzene	C <sub>6</sub> H <sub>12</sub>	-4.05	-4.20
0035ben	benzene	C <sub>6</sub> H <sub>6</sub>	-4.55	-4.79
0036tol	benzene	C <sub>7</sub> H <sub>8</sub>	-5.32	-5.52
0044met	benzene	CH <sub>4</sub> O	-2.58	-2.36
0045eth	benzene	C <sub>2</sub> H <sub>6</sub> O	-3.42	-3.17
0047pro	benzene	C <sub>3</sub> H <sub>8</sub> O	-3.87	-4.00
0048pro	benzene	C <sub>3</sub> H <sub>8</sub> O	-3.48	-3.71
0049but	benzene	C <sub>4</sub> H <sub>10</sub> O	-4.45	-4.77
0050met	benzene	C <sub>4</sub> H <sub>10</sub> O	-3.70	-4.53
0052pen	benzene	C <sub>5</sub> H <sub>12</sub> O	-5.10	-5.40
0053phe	benzene	C <sub>6</sub> H <sub>6</sub> O	-7.12	-6.46
0054hex	benzene	C <sub>6</sub> H <sub>14</sub> O	-6.13	-6.13
0055ocr	benzene	C <sub>7</sub> H <sub>8</sub> O	-7.44	-7.23
0056mcr	benzene	C <sub>7</sub> H <sub>8</sub> O	-6.66	-7.23
0057pcr	benzene	C <sub>7</sub> H <sub>8</sub> O	-7.35	-7.22
0058hep	benzene	C <sub>7</sub> H <sub>16</sub> O	-6.85	-6.86
0062dio	benzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.21	-5.05
0075pro	benzene	C <sub>3</sub> H <sub>6</sub> O	-3.79	-3.83
0076but	benzene	C <sub>4</sub> H <sub>8</sub> O	-4.46	-4.51
0078pen	benzene	C <sub>5</sub> H <sub>10</sub> O	-5.14	-5.18
0080hex	benzene	C <sub>6</sub> H <sub>12</sub> O	-5.76	-5.84
0082hep	benzene	C <sub>7</sub> H <sub>14</sub> O	-6.36	-6.49
0086eth	benzene	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-4.02	-4.34
0087pro	benzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.75	-4.91
0088but	benzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.30	-5.49
0089pen	benzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-6.01	-6.05
0090hex	benzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-6.94	-6.72
0093met	benzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.04	-4.37
0094met	benzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.58	-4.76
0095eth	benzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.53	-4.83
0097pro	benzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-5.21	-5.39
0098met	benzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.83	-6.04
0099but	benzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.78	-6.03
0100met	benzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.47	-6.68
0101pen	benzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.53	-6.67
0103eth	benzene	C <sub>2</sub> H <sub>7</sub> N	-2.73	-2.57
0104dim	benzene	C <sub>2</sub> H <sub>7</sub> N	-3.01	-2.79
0106pro	benzene	C <sub>3</sub> H <sub>9</sub> N	-3.68	-3.30
0107tri	benzene	C <sub>3</sub> H <sub>9</sub> N	-2.80	-3.03
0111die	benzene	C <sub>4</sub> H <sub>11</sub> N	-4.02	-3.90
0115dip	benzene	C <sub>6</sub> H <sub>15</sub> N	-5.09	-5.14
0116pyr	benzene	C <sub>5</sub> H <sub>5</sub> N	-5.28	-5.31
0118ani	benzene	C <sub>6</sub> H <sub>7</sub> N	-6.88	-6.90
0119met	benzene	C <sub>6</sub> H <sub>7</sub> N	-5.86	-6.04
0121met	benzene	C <sub>6</sub> H <sub>7</sub> N	-6.17	-6.06
0122Nme	benzene	C <sub>7</sub> H <sub>9</sub> N	-6.64	-6.98

0125dim	benzene	C <sub>7</sub> H <sub>9</sub> N	-6.39	-6.70
0134nit	benzene	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-7.60	-7.38
0150mhy	benzene	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-9.29	-8.53
0151phy	benzene	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-9.73	-8.58
0215pbr	benzene	C <sub>6</sub> H <sub>5</sub> OBr	-8.81	-8.50
0216amm	benzene	H <sub>3</sub> N	-1.12	-1.63
0217wat	benzene	H <sub>2</sub> O	-1.71	-2.17
0220tri	benzene	C <sub>3</sub> H <sub>9</sub> O <sub>4</sub> P	-8.02	-6.30
0221tri	benzene	C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P	-8.58	-7.38
0222tri	benzene	C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> P	-9.34	-8.64
0225pipa	benzene	C <sub>5</sub> H <sub>11</sub> N	-5.03	-5.31
0228met	benzene	CH <sub>3</sub> N	-2.66	-2.08
0229hyd	benzene	H <sub>4</sub> N <sub>2</sub>	-4.02	-2.21
0236oct	benzene	C <sub>8</sub> H <sub>18</sub> O	-8.06	-7.59
0240met	benzene	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-6.27	-7.79
0401amia	benzene	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O	-12.18	-11.93
0433pho	benzene	C <sub>4</sub> H <sub>7</sub> O <sub>4</sub> PCl <sub>2</sub>	-9.09	-8.33
0441pho	benzene	C <sub>8</sub> H <sub>10</sub> NO <sub>3</sub> PS	-9.21	-11.37
0447pho	benzene	C <sub>10</sub> H <sub>14</sub> NO <sub>3</sub> PS	-8.58	-12.80
0506nit	benzene	CH <sub>3</sub> NO <sub>2</sub>	-4.50	-4.27
0571dim	benzene	C <sub>7</sub> H <sub>9</sub> N	-7.64	-6.76
n008	benzene	C <sub>7</sub> H <sub>7</sub> NO	-9.93	-9.86
n009	benzene	C <sub>7</sub> H <sub>9</sub> N	-7.37	-7.41
n010	benzene	C <sub>7</sub> H <sub>9</sub> N	-7.61	-7.59
n011	benzene	C <sub>7</sub> H <sub>9</sub> N	-7.59	-7.60
0093met	sec-butylbenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.91	-3.32
0095eth	sec-butylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.11	-3.73
0097pro	sec-butylbenzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.62	-4.37
0099but	sec-butylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.22	-5.08
0101pen	sec-butylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.98	-5.80
0076but	tert-butylbenzene	C <sub>4</sub> H <sub>8</sub> O	-3.94	-3.79
0078pen	tert-butylbenzene	C <sub>5</sub> H <sub>10</sub> O	-4.72	-4.53
0080hex	tert-butylbenzene	C <sub>6</sub> H <sub>12</sub> O	-5.27	-5.28
0081dim	tert-butylbenzene	C <sub>6</sub> H <sub>12</sub> O	-4.79	-4.47
0082hep	tert-butylbenzene	C <sub>7</sub> H <sub>14</sub> O	-5.88	-6.01
0093met	tert-butylbenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.57	-3.46
0094met	tert-butylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.17	-3.77
0095eth	tert-butylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.22	-3.86
0097pro	tert-butylbenzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.72	-4.49
0098met	tert-butylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.39	-5.24
0099but	tert-butylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.25	-5.21
0100met	tert-butylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.13	-5.98
0101pen	tert-butylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.92	-5.92
0530tibu	tert-butylbenzene	C <sub>10</sub> H <sub>14</sub>	-6.43	-6.67
0053phe	butylbenzene	C <sub>6</sub> H <sub>6</sub> O	-6.76	-6.01
0078pen	butylbenzene	C <sub>5</sub> H <sub>10</sub> O	-4.74	-4.23
0080hex	butylbenzene	C <sub>6</sub> H <sub>12</sub> O	-5.31	-4.99
0081dim	butylbenzene	C <sub>6</sub> H <sub>12</sub> O	-4.77	-4.15
0082hep	butylbenzene	C <sub>7</sub> H <sub>14</sub> O	-5.93	-5.74
0094met	butylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.19	-3.49
0098met	butylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.37	-4.99
0099but	butylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.28	-4.96
0100met	butylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.09	-5.74
0529but	butylbenzene	C <sub>10</sub> H <sub>14</sub>	-6.86	-6.82
0076but	trimethylbenzene	C <sub>4</sub> H <sub>8</sub> O	-3.97	-3.64
0078pen	trimethylbenzene	C <sub>5</sub> H <sub>10</sub> O	-4.83	-4.39
0080hex	trimethylbenzene	C <sub>6</sub> H <sub>12</sub> O	-5.39	-5.15
0081dim	trimethylbenzene	C <sub>6</sub> H <sub>12</sub> O	-4.80	-4.40
0082hep	trimethylbenzene	C <sub>7</sub> H <sub>14</sub> O	-6.01	-5.90
0093met	trimethylbenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.58	-3.36
0094met	trimethylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.14	-3.73
0098met	trimethylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.41	-5.19
0100met	trimethylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.16	-5.91
0101pen	trimethylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.09	-5.90
0532tri	trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	-6.47	-6.28
0045eth	isopropylbenzene	C <sub>2</sub> H <sub>6</sub> O	-2.90	-2.95
0075pro	isopropylbenzene	C <sub>3</sub> H <sub>6</sub> O	-3.32	-3.15
0076but	isopropylbenzene	C <sub>4</sub> H <sub>8</sub> O	-4.02	-3.81
0078pen	isopropylbenzene	C <sub>5</sub> H <sub>10</sub> O	-4.84	-4.58
0080hex	isopropylbenzene	C <sub>6</sub> H <sub>12</sub> O	-5.39	-5.33
0081dim	isopropylbenzene	C <sub>6</sub> H <sub>12</sub> O	-4.81	-4.59
0082hep	isopropylbenzene	C <sub>7</sub> H <sub>14</sub> O	-5.99	-6.01
0087pro	isopropylbenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.23	-4.65
0088but	isopropylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.93	-5.35
0094met	isopropylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.19	-3.88
0095eth	isopropylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.22	-3.97
0097pro	isopropylbenzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.78	-4.59
0098met	isopropylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.45	-5.30
0099but	isopropylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.36	-5.31
0100met	isopropylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.19	-6.01
0101pen	isopropylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.13	-6.01
0110but	isopropylbenzene	C <sub>4</sub> H <sub>11</sub> N	-4.06	-3.93
0217wat	isopropylbenzene	H <sub>2</sub> O	-1.41	-1.96

0502pro	isopropylbenzene	C <sub>9</sub> H <sub>12</sub>	-6.04	-6.36
0008noc	toluene	C <sub>8</sub> H <sub>18</sub>	-5.38	-5.37
0036tol	toluene	C <sub>7</sub> H <sub>8</sub>	-5.12	-5.31
0044met	toluene	CH <sub>4</sub> O	-2.18	-2.22
0045eth	toluene	C <sub>2</sub> H <sub>6</sub> O	-3.33	-3.02
0047pro	toluene	C <sub>3</sub> H <sub>8</sub> O	-3.71	-3.84
0049but	toluene	C <sub>4</sub> H <sub>10</sub> O	-4.31	-4.65
0052pen	toluene	C <sub>5</sub> H <sub>12</sub> O	-5.17	-5.39
0053phe	toluene	C <sub>6</sub> H <sub>6</sub> O	-6.93	-6.37
0054hex	toluene	C <sub>6</sub> H <sub>14</sub> O	-6.12	-6.16
0055ocr	toluene	C <sub>7</sub> H <sub>8</sub> O	-7.43	-7.13
0057pcr	toluene	C <sub>7</sub> H <sub>8</sub> O	-7.56	-7.12
0058hep	toluene	C <sub>7</sub> H <sub>16</sub> O	-6.75	-6.89
0062dio	toluene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.91	-4.83
0075pro	toluene	C <sub>3</sub> H <sub>6</sub> O	-3.59	-3.59
0076but	toluene	C <sub>4</sub> H <sub>8</sub> O	-4.27	-4.27
0078pen	toluene	C <sub>5</sub> H <sub>10</sub> O	-5.02	-4.94
0080hex	toluene	C <sub>6</sub> H <sub>12</sub> O	-5.60	-5.60
0081dim	toluene	C <sub>6</sub> H <sub>12</sub> O	-5.00	-5.06
0082hep	toluene	C <sub>7</sub> H <sub>14</sub> O	-6.30	-6.25
0086eth	toluene	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-4.00	-4.23
0087pro	toluene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.57	-4.79
0088but	toluene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.24	-5.43
0089pen	toluene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-5.89	-6.07
0090hex	toluene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-6.97	-6.78
0093met	toluene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.81	-3.98
0094met	toluene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.62	-4.35
0095eth	toluene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.41	-4.44
0097pro	toluene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-5.00	-5.07
0098met	toluene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.65	-5.78
0099but	toluene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.57	-5.78
0100met	toluene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.38	-6.44
0101pen	toluene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.41	-6.42
0103eth	toluene	C <sub>2</sub> H <sub>7</sub> N	-2.67	-2.61
0104dim	toluene	C <sub>2</sub> H <sub>7</sub> N	-2.68	-2.77
0106pro	toluene	C <sub>3</sub> H <sub>9</sub> N	-3.51	-3.33
0107tri	toluene	C <sub>3</sub> H <sub>9</sub> N	-2.71	-2.92
0110but	toluene	C <sub>4</sub> H <sub>11</sub> N	-4.33	-4.06
0111die	toluene	C <sub>4</sub> H <sub>11</sub> N	-3.75	-3.90
0115dip	toluene	C <sub>6</sub> H <sub>15</sub> N	-5.24	-5.14
0116pyr	toluene	C <sub>5</sub> H <sub>5</sub> N	-5.13	-5.12
0118ani	toluene	C <sub>6</sub> H <sub>7</sub> N	-6.69	-6.66
0131nit	toluene	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-5.25	-5.36
0215pbr	toluene	C <sub>6</sub> H <sub>5</sub> OBr	-8.70	-8.51
0216amm	toluene	H <sub>3</sub> N	-2.38	-1.42
0217wat	toluene	H <sub>2</sub> O	-1.69	-2.06
0228met	toluene	CH <sub>3</sub> N	-2.65	-2.01
0240met	toluene	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-7.96	-7.58
0506nit	toluene	CH <sub>3</sub> NO <sub>2</sub>	-4.31	-4.11
0648gbu	toluene	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	-4.70	-5.90
n011	toluene	C <sub>7</sub> H <sub>9</sub> N	-7.39	-7.45
0008noc	triethylamine	C <sub>8</sub> H <sub>18</sub>	-5.62	-5.34
0036tol	triethylamine	C <sub>7</sub> H <sub>8</sub>	-4.98	-4.97
0045eth	triethylamine	C <sub>2</sub> H <sub>6</sub> O	-4.02	-3.73
0062dio	triethylamine	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.41	-4.46
0076but	triethylamine	C <sub>4</sub> H <sub>8</sub> O	-3.86	-3.70
0506nit	triethylamine	CH <sub>3</sub> NO <sub>2</sub>	-3.63	-2.74
0510tri	triethylamine	C <sub>6</sub> H <sub>15</sub> N	-4.44	-4.27
0008noc	xylene	C <sub>8</sub> H <sub>18</sub>	-5.29	-5.30
0036tol	xylene	C <sub>7</sub> H <sub>8</sub>	-5.06	-5.07
0044met	xylene	CH <sub>4</sub> O	-1.73	-2.13
0045eth	xylene	C <sub>2</sub> H <sub>6</sub> O	-3.42	-2.93
0047pro	xylene	C <sub>3</sub> H <sub>8</sub> O	-3.57	-3.73
0049but	xylene	C <sub>4</sub> H <sub>10</sub> O	-4.17	-4.55
0052pen	xylene	C <sub>5</sub> H <sub>12</sub> O	-4.72	-5.28
0053phe	xylene	C <sub>6</sub> H <sub>6</sub> O	-6.83	-6.20
0054hex	xylene	C <sub>6</sub> H <sub>14</sub> O	-5.85	-6.07
0055ocr	xylene	C <sub>7</sub> H <sub>8</sub> O	-7.25	-6.98
0056mcr	xylene	C <sub>7</sub> H <sub>8</sub> O	-6.32	-6.97
0057pcr	xylene	C <sub>7</sub> H <sub>8</sub> O	-7.18	-6.97
0058hep	xylene	C <sub>7</sub> H <sub>16</sub> O	-6.74	-6.87
0062dio	xylene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.86	-4.63
0075pro	xylene	C <sub>3</sub> H <sub>6</sub> O	-3.26	-3.25
0076but	xylene	C <sub>4</sub> H <sub>8</sub> O	-4.23	-3.90
0078pen	xylene	C <sub>5</sub> H <sub>10</sub> O	-4.87	-4.65
0080hex	xylene	C <sub>6</sub> H <sub>12</sub> O	-5.49	-5.38
0081dim	xylene	C <sub>6</sub> H <sub>12</sub> O	-4.91	-4.67
0082hep	xylene	C <sub>7</sub> H <sub>14</sub> O	-6.15	-6.04
0086eth	xylene	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-4.08	-3.98
0087pro	xylene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.72	-4.61
0088but	xylene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.30	-5.34
0089pen	xylene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-5.71	-6.04
0090hex	xylene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-6.67	-6.82



0093met	xylene	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	-3.70	-3.62
0094met	xylene	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-4.20	-4.00
0095eth	xylene	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-4.26	-4.07
0097pro	xylene	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	-4.87	-4.73
0098met	xylene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.61	-5.46
0099but	xylene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.40	-5.45
0100met	xylene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.26	-6.18
0101pen	xylene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.19	-6.17
0103eth	xylene	C <sub>2</sub> H <sub>7</sub> N	-3.01	-2.50
0104dim	xylene	C <sub>2</sub> H <sub>7</sub> N	-3.36	-2.66
0106pro	xylene	C <sub>3</sub> H <sub>9</sub> N	-3.69	-3.26
0107tri	xylene	C <sub>3</sub> H <sub>9</sub> N	-2.63	-2.83
0111die	xylene	C <sub>4</sub> H <sub>11</sub> N	-3.93	-3.88
0113pen	xylene	C <sub>5</sub> H <sub>13</sub> N	-4.70	-4.77
0115dip	xylene	C <sub>6</sub> H <sub>15</sub> N	-5.35	-5.13
0116pyr	xylene	C <sub>5</sub> H <sub>5</sub> N	-5.12	-4.88
0118ani	xylene	C <sub>6</sub> H <sub>7</sub> N	-6.10	-6.37
0215pbr	xylene	C <sub>6</sub> H <sub>5</sub> OBr	-8.69	-8.45
0217wat	xylene	H <sub>2</sub> O	-1.56	-1.96
0225pipa	xylene	C <sub>3</sub> H <sub>11</sub> N	-5.15	-5.29
0228met	xylene	CH <sub>3</sub> N	-3.20	-1.90
0506nit	xylene	CH <sub>3</sub> NO <sub>2</sub>	-4.20	-3.90
n011	xylene	C <sub>7</sub> H <sub>9</sub> N	-7.17	-7.16
0037eth	ethylbenzene	C <sub>8</sub> H <sub>10</sub>	-5.67	-5.83
0044met	ethylbenzene	CH <sub>4</sub> O	-1.43	-2.19
0045eth	ethylbenzene	C <sub>2</sub> H <sub>6</sub> O	-2.49	-2.98
0047pro	ethylbenzene	C <sub>3</sub> H <sub>8</sub> O	-3.71	-3.78
0049but	ethylbenzene	C <sub>4</sub> H <sub>10</sub> O	-3.77	-4.60
0052pen	ethylbenzene	C <sub>5</sub> H <sub>12</sub> O	-4.72	-5.33
0053phe	ethylbenzene	C <sub>6</sub> H <sub>6</sub> O	-6.82	-6.30
0054hex	ethylbenzene	C <sub>6</sub> H <sub>14</sub> O	-5.68	-6.12
0055ocr	ethylbenzene	C <sub>7</sub> H <sub>8</sub> O	-7.25	-7.06
0058hep	ethylbenzene	C <sub>7</sub> H <sub>16</sub> O	-6.70	-6.92
0075pro	ethylbenzene	C <sub>3</sub> H <sub>6</sub> O	-3.41	-3.31
0076but	ethylbenzene	C <sub>4</sub> H <sub>8</sub> O	-4.12	-3.96
0078pen	ethylbenzene	C <sub>5</sub> H <sub>10</sub> O	-4.85	-4.71
0080hex	ethylbenzene	C <sub>6</sub> H <sub>12</sub> O	-5.49	-5.41
0081dim	ethylbenzene	C <sub>6</sub> H <sub>12</sub> O	-4.92	-4.75
0082hep	ethylbenzene	C <sub>7</sub> H <sub>14</sub> O	-6.10	-6.07
0093met	ethylbenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.74	-3.69
0094met	ethylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.29	-4.03
0095eth	ethylbenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.31	-4.12
0097pro	ethylbenzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.95	-4.76
0098met	ethylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.56	-5.49
0099but	ethylbenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.48	-5.49
0101pen	ethylbenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.20	-6.21
0103eth	ethylbenzene	C <sub>2</sub> H <sub>7</sub> N	-2.59	-2.55
0106pro	ethylbenzene	C <sub>3</sub> H <sub>9</sub> N	-3.44	-3.31
0107tri	ethylbenzene	C <sub>3</sub> H <sub>9</sub> N	-2.64	-2.87
0110but	ethylbenzene	C <sub>4</sub> H <sub>11</sub> N	-4.43	-4.04
0215pbr	ethylbenzene	C <sub>6</sub> H <sub>5</sub> OBr	-8.54	-8.54
0217wat	ethylbenzene	H <sub>2</sub> O	-1.51	-2.04
0008noc	carbon disulfide	C <sub>8</sub> H <sub>18</sub>	-5.68	-5.52
0036tol	carbon disulfide	C <sub>7</sub> H <sub>8</sub>	-5.39	-5.42
0045eth	carbon disulfide	C <sub>2</sub> H <sub>6</sub> O	-2.72	-3.15
0053phe	carbon disulfide	C <sub>6</sub> H <sub>6</sub> O	-6.27	-6.22
0062dio	carbon disulfide	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.67	-5.27
0075pro	carbon disulfide	C <sub>3</sub> H <sub>6</sub> O	-3.14	-3.86
0076but	carbon disulfide	C <sub>4</sub> H <sub>8</sub> O	-3.85	-4.60
0086eth	carbon disulfide	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-2.98	-4.14
0093met	carbon disulfide	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.67	-4.35
0095eth	carbon disulfide	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.08	-4.89
0097pro	carbon disulfide	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.63	-5.50
0131nit	carbon disulfide	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-4.50	-5.36
0506nit	carbon disulfide	CH <sub>3</sub> NO <sub>2</sub>	-3.30	-4.00
0537car	carbon disulfide	C <sub>1</sub> S <sub>2</sub>	-3.95	-3.62
0045eth	tetralin	C <sub>2</sub> H <sub>6</sub> O	-1.54	-3.21
0075pro	tetralin	C <sub>3</sub> H <sub>8</sub> O	-2.54	-3.31
0076but	tetralin	C <sub>4</sub> H <sub>8</sub> O	-3.12	-3.95
0078pen	tetralin	C <sub>5</sub> H <sub>10</sub> O	-3.99	-4.55
0080hex	tetralin	C <sub>6</sub> H <sub>12</sub> O	-4.64	-5.24
0081dim	tetralin	C <sub>6</sub> H <sub>12</sub> O	-4.19	-4.69
0082hep	tetralin	C <sub>7</sub> H <sub>14</sub> O	-5.33	-5.97
0217wat	tetralin	H <sub>2</sub> O	0.07	-2.49
0534tet	tetralin	C <sub>10</sub> H <sub>12</sub>	-7.55	-7.69
0008noc	dibutyl ether	C <sub>8</sub> H <sub>18</sub>	-5.24	-5.26
0036tol	dibutyl ether	C <sub>7</sub> H <sub>8</sub>	-4.87	-4.96
0045eth	dibutyl ether	C <sub>2</sub> H <sub>6</sub> O	-3.51	-3.80
0062dio	dibutyl ether	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.37	-4.54
0076but	dibutyl ether	C <sub>4</sub> H <sub>8</sub> O	-3.78	-3.70
0086eth	dibutyl ether	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-5.21	-4.84
0087pro	dibutyl ether	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-6.11	-5.62
0111die	dibutyl ether	C <sub>4</sub> H <sub>11</sub> N	-3.80	-3.88

0116pyr	dibutyl ether	C <sub>8</sub> H <sub>18</sub> N	-4.65	-5.11
0117met	dibutyl ether	C <sub>8</sub> H <sub>16</sub> N <sub>2</sub>	-5.12	-6.45
0119met	dibutyl ether	C <sub>8</sub> H <sub>7</sub> N	-5.20	-5.79
0230eth	dibutyl ether	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub>	-5.87	-7.36
0501but	dibutyl ether	C <sub>8</sub> H <sub>18</sub> O	-5.76	-6.08
0506nit	dibutyl ether	CH <sub>3</sub> NO <sub>2</sub>	-3.67	-2.83
0008noc	diisopropyl ether	C <sub>8</sub> H <sub>18</sub>	-5.38	-5.41
0036tol	diisopropyl ether	C <sub>7</sub> H <sub>8</sub>	-4.91	-5.23
0041nap	diisopropyl ether	C <sub>10</sub> H <sub>8</sub>	-7.24	-7.39
0045eth	diisopropyl ether	C <sub>2</sub> H <sub>6</sub> O	-3.90	-4.30
0053phe	diisopropyl ether	C <sub>6</sub> H <sub>6</sub> O	-8.35	-7.55
0062dio	diisopropyl ether	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.42	-4.74
0069met	diisopropyl ether	CH <sub>2</sub> O	-1.04	-2.26
0076but	diisopropyl ether	C <sub>4</sub> H <sub>8</sub> O	-3.96	-4.29
0086eth	diisopropyl ether	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-5.73	-5.55
0087pro	diisopropyl ether	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-6.37	-6.32
0088but	diisopropyl ether	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-6.85	-6.93
0089pen	diisopropyl ether	C <sub>3</sub> H <sub>10</sub> O <sub>2</sub>	-7.59	-7.50
0090hex	diisopropyl ether	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-8.23	-8.13
0107tri	diisopropyl ether	C <sub>3</sub> H <sub>9</sub> N	-2.74	-3.24
0111die	diisopropyl ether	C <sub>4</sub> H <sub>11</sub> N	-3.78	-4.21
0116pyr	diisopropyl ether	C <sub>7</sub> H <sub>5</sub> N	-4.88	-5.72
0118ani	diisopropyl ether	C <sub>6</sub> H <sub>7</sub> N	-6.67	-7.55
0151phy	diisopropyl ether	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-11.63	-9.59
0217wat	diisopropyl ether	H <sub>2</sub> O	-3.58	-3.70
0242dii	diisopropyl ether	C <sub>6</sub> H <sub>14</sub> O	-3.97	-4.12
0506nit	diisopropyl ether	CH <sub>3</sub> NO <sub>2</sub>	-3.90	-3.40
0005npe	hexadecyl iodide	C <sub>8</sub> H <sub>12</sub>	-2.59	-2.03
0006nhe	hexadecyl iodide	C <sub>6</sub> H <sub>14</sub>	-3.26	-2.65
0007nhe	hexadecyl iodide	C <sub>7</sub> H <sub>16</sub>	-3.90	-3.36
0018cyc	hexadecyl iodide	C <sub>6</sub> H <sub>12</sub>	-3.66	-3.28
0019met	hexadecyl iodide	C <sub>7</sub> H <sub>14</sub>	-4.07	-3.80
0035ben	hexadecyl iodide	C <sub>6</sub> H <sub>6</sub>	-3.71	-2.96
0036tol	hexadecyl iodide	C <sub>7</sub> H <sub>8</sub>	-4.41	-3.63
0161dic	hexadecyl iodide	CH <sub>2</sub> Cl <sub>2</sub>	-2.76	-2.71
0162tri	hexadecyl iodide	CHCl <sub>3</sub>	-3.36	-3.35
0008noc	phenyl ether	C <sub>8</sub> H <sub>18</sub>	-4.38	-4.62
0036tol	phenyl ether	C <sub>7</sub> H <sub>8</sub>	-4.86	-5.20
0045eth	phenyl ether	C <sub>2</sub> H <sub>6</sub> O	-3.22	-4.04
0062dio	phenyl ether	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.83	-5.11
0076but	phenyl ether	C <sub>4</sub> H <sub>8</sub> O	-4.08	-4.71
0506nit	phenyl ether	CH <sub>3</sub> NO <sub>2</sub>	-4.19	-5.19
0093met	fluorooctane	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-3.59	-3.52
0094met	fluorooctane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.09	-4.17
0095eth	fluorooctane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.16	-4.09
0097pro	fluorooctane	C <sub>3</sub> H <sub>10</sub> O <sub>2</sub>	-4.65	-4.76
0098met	fluorooctane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.33	-5.66
0099but	fluorooctane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.22	-5.50
0008noc	ethoxybenzene	C <sub>8</sub> H <sub>18</sub>	-4.75	-4.76
0036tol	ethoxybenzene	C <sub>7</sub> H <sub>8</sub>	-4.99	-4.98
0045eth	ethoxybenzene	C <sub>2</sub> H <sub>6</sub> O	-3.45	-4.05
0062dio	ethoxybenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.87	-4.55
0076but	ethoxybenzene	C <sub>4</sub> H <sub>8</sub> O	-4.28	-4.09
0246eth	ethoxybenzene	C <sub>8</sub> H <sub>10</sub> O	-6.75	-7.06
0506nit	ethoxybenzene	CH <sub>3</sub> NO <sub>2</sub>	-4.45	-4.58
0008noc	anisole	C <sub>8</sub> H <sub>18</sub>	-4.62	-4.73
0036tol	anisole	C <sub>7</sub> H <sub>8</sub>	-4.95	-5.05
0045eth	anisole	C <sub>2</sub> H <sub>6</sub> O	-3.59	-4.12
0062dio	anisole	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.06	-4.62
0068ani	anisole	C <sub>7</sub> H <sub>8</sub> O	-6.33	-6.46
0076but	anisole	C <sub>4</sub> H <sub>8</sub> O	-4.43	-4.22
0110but	anisole	C <sub>4</sub> H <sub>11</sub> N	-4.44	-4.67
0506nit	anisole	CH <sub>3</sub> NO <sub>2</sub>	-4.69	-4.72
0008noc	diethyl ether	C <sub>8</sub> H <sub>18</sub>	-5.62	-5.32
0035ben	diethyl ether	C <sub>6</sub> H <sub>6</sub>	-4.21	-4.68
0036tol	diethyl ether	C <sub>7</sub> H <sub>8</sub>	-5.23	-5.23
0037eth	diethyl ether	C <sub>8</sub> H <sub>10</sub>	-5.45	-5.94
0038oxy	diethyl ether	C <sub>6</sub> H <sub>10</sub>	-5.58	-5.73
0039mxy	diethyl ether	C <sub>8</sub> H <sub>10</sub>	-5.56	-5.76
0041nap	diethyl ether	C <sub>10</sub> H <sub>8</sub>	-7.25	-7.52
0044met	diethyl ether	CH <sub>4</sub> O	-3.61	-3.85
0045eth	diethyl ether	C <sub>2</sub> H <sub>6</sub> O	-4.41	-4.55
0046eth	diethyl ether	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	-6.20	-5.88
0047pro	diethyl ether	C <sub>3</sub> H <sub>8</sub> O	-4.90	-5.22
0048pro	diethyl ether	C <sub>3</sub> H <sub>8</sub> O	-4.44	-4.74
0049but	diethyl ether	C <sub>4</sub> H <sub>10</sub> O	-5.69	-5.87
0050met	diethyl ether	C <sub>4</sub> H <sub>10</sub> O	-4.80	-4.52
0051cyc	diethyl ether	C <sub>5</sub> H <sub>10</sub> O	-6.50	-6.55
0052pen	diethyl ether	C <sub>3</sub> H <sub>12</sub> O	-6.11	-6.41
0053phe	diethyl ether	C <sub>6</sub> H <sub>6</sub> O	-8.75	-7.88
0054hex	diethyl ether	C <sub>6</sub> H <sub>14</sub> O	-6.82	-7.06
0056mcr	diethyl ether	C <sub>7</sub> H <sub>8</sub> O	-7.95	-8.39
0058hep	diethyl ether	C <sub>7</sub> H <sub>16</sub> O	-7.51	-7.71

0062dio	diethyl ether	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.67	-4.66
0063die	diethyl ether	C <sub>4</sub> H <sub>10</sub> O	-3.39	-3.48
0068ani	diethyl ether	C <sub>7</sub> H <sub>8</sub> O	-5.71	-6.08
0070eth	diethyl ether	C <sub>2</sub> H <sub>4</sub> O	-2.85	-3.04
0071proa	diethyl ether	C <sub>3</sub> H <sub>6</sub> O	-3.85	-3.92
0074ben	diethyl ether	C <sub>7</sub> H <sub>6</sub> O	-6.08	-6.93
0076but	diethyl ether	C <sub>4</sub> H <sub>8</sub> O	-4.09	-4.50
0084met	diethyl ether	C <sub>6</sub> H <sub>8</sub> O	-6.79	-7.53
0086eth	diethyl ether	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-6.26	-5.87
0087pro	diethyl ether	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-6.75	-6.66
0088but	diethyl ether	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-7.32	-7.27
0089pen	diethyl ether	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-7.87	-7.84
0090hex	diethyl ether	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-8.85	-8.45
0103eth	diethyl ether	C <sub>2</sub> H <sub>7</sub> N	-2.89	-3.71
0104dim	diethyl ether	C <sub>2</sub> H <sub>7</sub> N	-2.63	-3.66
0106pro	diethyl ether	C <sub>3</sub> H <sub>9</sub> N	-3.65	-4.27
0107tri	diethyl ether	C <sub>3</sub> H <sub>9</sub> N	-2.78	-3.21
0110but	diethyl ether	C <sub>4</sub> H <sub>11</sub> N	-4.24	-4.86
0111die	diethyl ether	C <sub>4</sub> H <sub>11</sub> N	-3.83	-4.22
0115dip	diethyl ether	C <sub>6</sub> H <sub>15</sub> N	-4.96	-5.29
0116pyr	diethyl ether	C <sub>5</sub> H <sub>5</sub> N	-4.81	-5.87
0118ani	diethyl ether	C <sub>6</sub> H <sub>7</sub> N	-6.51	-7.75
0126eth	diethyl ether	C <sub>2</sub> H <sub>3</sub> N	-3.59	-3.94
0129ben	diethyl ether	C <sub>7</sub> H <sub>5</sub> N	-6.36	-8.10
0134nit	diethyl ether	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-6.85	-7.26
0135met	diethyl ether	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	-7.21	-8.11
0145pro	diethyl ether	C <sub>3</sub> H <sub>6</sub> O	-4.87	-5.60
0146met	diethyl ether	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	-5.12	-5.60
0150mhy	diethyl ether	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-11.36	-9.95
0151phy	diethyl ether	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-12.07	-10.02
0174chl	diethyl ether	C <sub>6</sub> H <sub>5</sub> Cl	-5.42	-6.03
0176pdi	diethyl ether	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-6.18	-7.23
0186bro	diethyl ether	C <sub>6</sub> H <sub>5</sub> Br	-5.99	-6.18
0216amm	diethyl ether	H <sub>3</sub> N	-1.41	-2.33
0217wat	diethyl ether	H <sub>2</sub> O	-3.85	-3.99
0219hyd	diethyl ether	H <sub>2</sub> S	-0.60	-2.00
0225pipa	diethyl ether	C <sub>3</sub> H <sub>11</sub> N	-4.82	-5.76
0228met	diethyl ether	CH <sub>3</sub> N	-2.32	-3.48
0229hyd	diethyl ether	H <sub>4</sub> N <sub>2</sub>	-3.08	-2.95
0233ethb	diethyl ether	C <sub>2</sub> H <sub>5</sub> NO	-6.16	-7.02
0236oct	diethyl ether	C <sub>8</sub> H <sub>18</sub> O	-7.25	-8.36
0506nit	diethyl ether	CH <sub>3</sub> NO <sub>2</sub>	-4.19	-3.90
0515dim	diethyl ether	C <sub>3</sub> H <sub>7</sub> NO	-5.31	-5.78
n007	diethyl ether	CH <sub>4</sub> N <sub>2</sub> O	-9.11	-6.23
n008	diethyl ether	C <sub>7</sub> H <sub>7</sub> NO	-10.60	-10.56
n127	diethyl ether	CH <sub>3</sub> NO	-5.97	-6.47
n191	diethyl ether	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	-15.03	-10.02
n200	diethyl ether	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> F	-15.56	-11.18
n203	diethyl ether	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> Br	-17.01	-10.91
test4001	diethyl ether	C <sub>6</sub> H <sub>5</sub> I	-6.64	-6.91
test4003	diethyl ether	CH <sub>3</sub> I	-3.51	-3.18
0044met	bromoform	CH <sub>4</sub> O	-2.79	-2.23
0045eth	bromoform	C <sub>2</sub> H <sub>6</sub> O	-3.24	-3.10
0047pro	bromoform	C <sub>3</sub> H <sub>8</sub> O	-4.03	-3.87
0049but	bromoform	C <sub>4</sub> H <sub>10</sub> O	-4.72	-4.67
0052pen	bromoform	C <sub>5</sub> H <sub>12</sub> O	-5.34	-5.35
0053phe	bromoform	C <sub>6</sub> H <sub>6</sub> O	-6.88	-6.56
0054hex	bromoform	C <sub>6</sub> H <sub>14</sub> O	-6.20	-6.12
0055ocr	bromoform	C <sub>7</sub> H <sub>8</sub> O	-7.45	-7.31
0058hep	bromoform	C <sub>7</sub> H <sub>16</sub> O	-7.10	-6.88
0086eth	bromoform	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-4.54	-4.03
0179tri	bromoform	CHBr <sub>3</sub>	-6.21	-6.61
0215pbr	bromoform	C <sub>6</sub> H <sub>5</sub> OBr	-8.49	-9.04
0008noc	iodobenzene	C <sub>8</sub> H <sub>18</sub>	-4.72	-4.71
0036tol	iodobenzene	C <sub>7</sub> H <sub>8</sub>	-4.99	-4.91
0044met	iodobenzene	CH <sub>4</sub> O	-2.18	-2.54
0045eth	iodobenzene	C <sub>2</sub> H <sub>6</sub> O	-3.18	-3.29
0047pro	iodobenzene	C <sub>3</sub> H <sub>8</sub> O	-3.52	-4.08
0049but	iodobenzene	C <sub>4</sub> H <sub>10</sub> O	-4.05	-4.88
0052pen	iodobenzene	C <sub>5</sub> H <sub>12</sub> O	-5.02	-5.56
0053phe	iodobenzene	C <sub>6</sub> H <sub>6</sub> O	-6.76	-6.78
0054hex	iodobenzene	C <sub>6</sub> H <sub>14</sub> O	-5.71	-6.33
0055ocr	iodobenzene	C <sub>7</sub> H <sub>8</sub> O	-7.14	-7.53
0056mcr	iodobenzene	C <sub>7</sub> H <sub>8</sub> O	-6.04	-7.52
0057pcr	iodobenzene	C <sub>7</sub> H <sub>8</sub> O	-7.01	-7.53
0058hep	iodobenzene	C <sub>7</sub> H <sub>16</sub> O	-6.53	-7.09
0062dio	iodobenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.94	-4.43
0076but	iodobenzene	C <sub>4</sub> H <sub>8</sub> O	-4.22	-4.08
0103eth	iodobenzene	C <sub>2</sub> H <sub>7</sub> N	-2.73	-2.68
0106pro	iodobenzene	C <sub>3</sub> H <sub>9</sub> N	-3.54	-3.40
0110but	iodobenzene	C <sub>4</sub> H <sub>11</sub> N	-4.19	-4.13
0215pbr	iodobenzene	C <sub>6</sub> H <sub>5</sub> OBr	-8.45	-9.26
0506nit	iodobenzene	CH <sub>3</sub> NO <sub>2</sub>	-4.10	-4.50

0008noc	chloroform	C <sub>8</sub> H <sub>18</sub>	-5.25	-5.25
0018cyc	chloroform	C <sub>6</sub> H <sub>12</sub>	-4.45	-4.35
0035ben	chloroform	C <sub>6</sub> H <sub>6</sub>	-4.64	-4.72
0036tol	chloroform	C <sub>7</sub> H <sub>8</sub>	-5.48	-5.36
0037eth	chloroform	C <sub>8</sub> H <sub>10</sub>	-5.84	-6.01
0038oxy	chloroform	C <sub>8</sub> H <sub>10</sub>	-6.23	-6.00
0039mxy	chloroform	C <sub>8</sub> H <sub>10</sub>	-5.86	-5.96
0041nap	chloroform	C <sub>10</sub> H <sub>8</sub>	-7.89	-7.90
0044met	chloroform	CH <sub>4</sub> O	-3.32	-2.91
0045eth	chloroform	C <sub>2</sub> H <sub>6</sub> O	-3.94	-3.82
0046eth	chloroform	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	-5.98	-5.57
0047pro	chloroform	C <sub>3</sub> H <sub>8</sub> O	-4.41	-4.64
0048pro	chloroform	C <sub>3</sub> H <sub>8</sub> O	-4.28	-4.26
0049but	chloroform	C <sub>4</sub> H <sub>10</sub> O	-5.28	-5.38
0050met	chloroform	C <sub>4</sub> H <sub>10</sub> O	-4.48	-4.77
0052pen	chloroform	C <sub>5</sub> H <sub>12</sub> O	-5.90	-5.98
0053phe	chloroform	C <sub>6</sub> H <sub>6</sub> O	-7.14	-7.05
0054hex	chloroform	C <sub>6</sub> H <sub>14</sub> O	-6.67	-6.68
0055ocr	chloroform	C <sub>7</sub> H <sub>8</sub> O	-7.55	-7.73
0056mcr	chloroform	C <sub>7</sub> H <sub>8</sub> O	-6.70	-7.65
0057pcr	chloroform	C <sub>7</sub> H <sub>8</sub> O	-7.59	-7.66
0058hep	chloroform	C <sub>7</sub> H <sub>16</sub> O	-7.53	-7.39
0062dio	chloroform	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-6.21	-5.21
0063die	chloroform	C <sub>4</sub> H <sub>10</sub> O	-4.32	-3.80
0068ani	chloroform	C <sub>7</sub> H <sub>8</sub> O	-6.24	-6.44
0069met	chloroform	CH <sub>2</sub> O	0.12	-2.30
0070eth	chloroform	C <sub>2</sub> H <sub>4</sub> O	-3.65	-3.29
0074ben	chloroform	C <sub>7</sub> H <sub>6</sub> O	-7.09	-7.12
0075pro	chloroform	C <sub>3</sub> H <sub>6</sub> O	-4.42	-4.00
0076but	chloroform	C <sub>4</sub> H <sub>8</sub> O	-5.43	-4.66
0084met	chloroform	C <sub>8</sub> H <sub>8</sub> O	-7.81	-7.90
0086eth	chloroform	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-4.74	-5.02
0087pro	chloroform	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-5.37	-5.77
0088but	chloroform	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.99	-6.44
0089pen	chloroform	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-6.61	-7.07
0090hex	chloroform	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-7.51	-7.69
0093met	chloroform	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.90	-4.43
0094met	chloroform	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.48	-4.84
0095eth	chloroform	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.58	-4.98
0097pro	chloroform	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-6.35	-5.59
0098met	chloroform	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-6.68	-6.24
0099but	chloroform	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-6.71	-6.21
0100met	chloroform	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-7.24	-6.89
0101pen	chloroform	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-7.36	-6.86
0103eth	chloroform	C <sub>2</sub> H <sub>7</sub> N	-4.02	-3.24
0104dim	chloroform	C <sub>2</sub> H <sub>7</sub> N	-3.69	-3.55
0106pro	chloroform	C <sub>3</sub> H <sub>9</sub> N	-4.73	-3.95
0107tri	chloroform	C <sub>3</sub> H <sub>9</sub> N	-3.90	-3.45
0111die	chloroform	C <sub>4</sub> H <sub>11</sub> N	-5.23	-4.38
0116pyr	chloroform	C <sub>5</sub> H <sub>5</sub> N	-6.45	-5.96
0117met	chloroform	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>	-6.99	-8.10
0118ani	chloroform	C <sub>6</sub> H <sub>7</sub> N	-7.34	-7.21
0119met	chloroform	C <sub>6</sub> H <sub>7</sub> N	-6.98	-6.84
0120met	chloroform	C <sub>6</sub> H <sub>7</sub> N	-7.35	-6.82
0121met	chloroform	C <sub>6</sub> H <sub>7</sub> N	-7.50	-6.82
0125dim	chloroform	C <sub>7</sub> H <sub>9</sub> N	-7.74	-7.59
0126eth	chloroform	C <sub>2</sub> H <sub>3</sub> N	-4.44	-4.54
0129ben	chloroform	C <sub>7</sub> H <sub>5</sub> N	-7.22	-8.25
0134nit	chloroform	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-7.78	-7.58
0135met	chloroform	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	-8.30	-8.47
0139thi	chloroform	C <sub>6</sub> H <sub>6</sub> S	-7.61	-7.79
0142die	chloroform	C <sub>4</sub> H <sub>10</sub> S	-6.40	-5.60
0144thi	chloroform	C <sub>7</sub> H <sub>6</sub> S	-5.98	-8.59
0145pro	chloroform	C <sub>3</sub> H <sub>6</sub> O	-4.34	-4.55
0149mor	chloroform	C <sub>4</sub> H <sub>9</sub> NO	-6.72	-7.60
0151phy	chloroform	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-10.30	-9.49
0157flu	chloroform	C <sub>6</sub> H <sub>5</sub> F	-4.25	-5.20
0162tri	chloroform	CHCl <sub>3</sub>	-4.13	-4.13
0174chl	chloroform	C <sub>6</sub> H <sub>5</sub> Cl	-5.45	-5.85
0176pdi	chloroform	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-6.32	-7.10
0186bro	chloroform	C <sub>6</sub> H <sub>5</sub> Br	-6.07	-6.19
0207tri	chloroform	C <sub>2</sub> H <sub>3</sub> OF <sub>3</sub>	-3.03	-3.14
0215pbr	chloroform	C <sub>6</sub> H <sub>5</sub> OBr	-8.59	-9.10
0216amm	chloroform	H <sub>3</sub> N	-2.41	-2.29
0217wat	chloroform	H <sub>2</sub> O	-2.05	-3.28
0219hyd	chloroform	H <sub>2</sub> S	-0.51	-1.84
0220tri	chloroform	C <sub>3</sub> H <sub>5</sub> O <sub>4</sub> P	-9.74	-7.77
0221tri	chloroform	C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P	-10.90	-9.04
0222tri	chloroform	C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> P	-11.11	-10.42
0225pipa	chloroform	C <sub>5</sub> H <sub>11</sub> N	-6.37	-6.25
0228met	chloroform	CH <sub>3</sub> N	-3.17	-2.93
0229hyd	chloroform	H <sub>4</sub> N <sub>2</sub>	-4.42	-3.02
0230eth	chloroform	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	-7.72	-8.74

0233ethb	chloroform	C <sub>2</sub> H <sub>5</sub> NO	-7.05	-7.37
0240met	chloroform	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-7.81	-8.09
0242dii	chloroform	C <sub>6</sub> H <sub>14</sub> O	-3.78	-4.75
0244tet	chloroform	C <sub>5</sub> H <sub>10</sub> O	-5.84	-5.29
0245thi	chloroform	C <sub>4</sub> H <sub>4</sub> S	-5.83	-5.33
0246eth	chloroform	C <sub>8</sub> H <sub>10</sub> O	-7.16	-7.07
0401amia	chloroform	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O	-13.64	-12.64
0402adn	chloroform	C <sub>6</sub> H <sub>7</sub> N <sub>5</sub>	-12.51	-16.16
0403thi	chloroform	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	-9.71	-12.30
0421dfl	chloroform	CF <sub>2</sub> Cl <sub>2</sub>	-1.55	-1.81
0422ffc	chloroform	CFCl <sub>3</sub>	-2.62	-3.25
0441pho	chloroform	C <sub>8</sub> H <sub>10</sub> NO <sub>5</sub> PS	-9.51	-10.41
0506nit	chloroform	CH <sub>3</sub> NO <sub>2</sub>	-4.68	-4.53
0519dim	chloroform	C <sub>4</sub> H <sub>9</sub> NO	-8.38	-6.95
0579pyy	chloroform	C <sub>4</sub> H <sub>5</sub> N	-5.50	-6.00
0582qui	chloroform	C <sub>9</sub> H <sub>7</sub> N	-10.23	-9.77
n007	chloroform	CH <sub>4</sub> N <sub>2</sub> O	-8.56	-7.18
n008	chloroform	C <sub>7</sub> H <sub>7</sub> NO	-11.06	-10.84
n009	chloroform	C <sub>7</sub> H <sub>9</sub> N	-8.23	-7.64
n011	chloroform	C <sub>7</sub> H <sub>9</sub> N	-8.01	-7.84
n186	chloroform	C <sub>5</sub> H <sub>9</sub> NO	-9.82	-8.07
n191	chloroform	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	-14.28	-10.99
n200	chloroform	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> F	-14.31	-11.91
n203	chloroform	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> Br	-15.03	-11.75
test4001	chloroform	C <sub>6</sub> H <sub>5</sub> I	-6.60	-7.15
0044met	dibromoethane	CH <sub>4</sub> O	-2.38	-2.40
0045eth	dibromoethane	C <sub>2</sub> H <sub>6</sub> O	-2.69	-3.27
0047pro	dibromoethane	C <sub>3</sub> H <sub>8</sub> O	-3.82	-4.09
0049but	dibromoethane	C <sub>4</sub> H <sub>10</sub> O	-4.65	-4.88
0052pen	dibromoethane	C <sub>5</sub> H <sub>12</sub> O	-5.44	-5.56
0053phe	dibromoethane	C <sub>6</sub> H <sub>6</sub> O	-7.22	-6.80
0054hex	dibromoethane	C <sub>6</sub> H <sub>14</sub> O	-6.08	-6.33
0057pcr	dibromoethane	C <sub>7</sub> H <sub>8</sub> O	-7.52	-7.55
0058hep	dibromoethane	C <sub>7</sub> H <sub>16</sub> O	-6.64	-7.09
0215pbr	dibromoethane	C <sub>6</sub> H <sub>5</sub> OBr	-9.01	-9.20
0041nap	butyl acetate	C <sub>10</sub> H <sub>8</sub>	-7.59	-7.47
0044met	butyl acetate	CH <sub>4</sub> O	-3.04	-3.29
0045eth	butyl acetate	C <sub>2</sub> H <sub>6</sub> O	-3.97	-3.97
0046eth	butyl acetate	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	-6.27	-5.78
0047pro	butyl acetate	C <sub>3</sub> H <sub>8</sub> O	-4.52	-4.72
0049but	butyl acetate	C <sub>4</sub> H <sub>10</sub> O	-5.23	-5.43
0052pen	butyl acetate	C <sub>5</sub> H <sub>12</sub> O	-5.78	-6.04
0053phe	butyl acetate	C <sub>6</sub> H <sub>6</sub> O	-8.96	-7.76
0054hex	butyl acetate	C <sub>6</sub> H <sub>14</sub> O	-6.62	-6.75
0055ocr	butyl acetate	C <sub>7</sub> H <sub>8</sub> O	-8.90	-8.22
0056mcr	butyl acetate	C <sub>7</sub> H <sub>8</sub> O	-8.44	-8.33
0057pcr	butyl acetate	C <sub>7</sub> H <sub>8</sub> O	-9.28	-8.38
0058hep	butyl acetate	C <sub>7</sub> H <sub>16</sub> O	-7.14	-7.46
0086eth	butyl acetate	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-6.11	-5.58
0099but	butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.52	-5.66
0116pyr	butyl acetate	C <sub>5</sub> H <sub>5</sub> N	-5.31	-5.56
0118ani	butyl acetate	C <sub>6</sub> H <sub>7</sub> N	-7.30	-7.88
0215pbr	butyl acetate	C <sub>6</sub> H <sub>5</sub> OBr	-10.57	-9.60
0217wat	butyl acetate	H <sub>2</sub> O	-4.13	-4.17
0236oct	butyl acetate	C <sub>8</sub> H <sub>18</sub> O	-8.17	-8.17
n011	butyl acetate	C <sub>7</sub> H <sub>9</sub> N	-7.81	-8.42
0093met	bromooctane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.35	-2.98
0095eth	bromooctane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-3.97	-3.58
0097pro	bromooctane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.48	-4.21
0099but	bromooctane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.11	-4.96
0101pen	bromooctane	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-5.81	-5.72
0008noc	bromobenzene	C <sub>8</sub> H <sub>18</sub>	-5.02	-4.91
0036tol	bromobenzene	C <sub>7</sub> H <sub>8</sub>	-5.13	-5.28
0044met	bromobenzene	CH <sub>4</sub> O	-2.31	-2.99
0045eth	bromobenzene	C <sub>2</sub> H <sub>6</sub> O	-3.26	-3.76
0047pro	bromobenzene	C <sub>3</sub> H <sub>8</sub> O	-3.74	-4.50
0049but	bromobenzene	C <sub>4</sub> H <sub>10</sub> O	-4.08	-5.28
0052pen	bromobenzene	C <sub>5</sub> H <sub>12</sub> O	-5.06	-5.96
0053phe	bromobenzene	C <sub>6</sub> H <sub>6</sub> O	-6.87	-7.24
0054hex	bromobenzene	C <sub>6</sub> H <sub>14</sub> O	-5.92	-6.72
0055ocr	bromobenzene	C <sub>7</sub> H <sub>8</sub> O	-7.26	-8.03
0057pcr	bromobenzene	C <sub>7</sub> H <sub>8</sub> O	-7.12	-8.02
0058hep	bromobenzene	C <sub>7</sub> H <sub>16</sub> O	-6.68	-7.48
0062dio	bromobenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.02	-4.88
0076but	bromobenzene	C <sub>4</sub> H <sub>8</sub> O	-4.37	-4.51
0093met	bromobenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.87	-4.23
0095eth	bromobenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.57	-4.58
0097pro	bromobenzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.93	-5.12
0099but	bromobenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.58	-5.79
0101pen	bromobenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.35	-6.51
0103eth	bromobenzene	C <sub>2</sub> H <sub>7</sub> N	-2.73	-3.07
0106pro	bromobenzene	C <sub>3</sub> H <sub>9</sub> N	-3.57	-3.78
0110but	bromobenzene	C <sub>4</sub> H <sub>11</sub> N	-4.22	-4.50

0118ani	bromobenzene	C <sub>6</sub> H <sub>7</sub> N	-6.66	-7.49
0186bro	bromobenzene	C <sub>6</sub> H <sub>5</sub> Br	-6.25	-6.19
0215pbr	bromobenzene	C <sub>6</sub> H <sub>5</sub> OBr	-8.49	-9.63
0506nit	bromobenzene	CH <sub>3</sub> NO <sub>2</sub>	-4.25	-4.99
n011	bromobenzene	C <sub>7</sub> H <sub>9</sub> N	-7.59	-8.26
0008noc	fluorobenzene	C <sub>6</sub> H <sub>18</sub>	-4.99	-5.16
0036tol	fluorobenzene	C <sub>7</sub> H <sub>8</sub>	-5.27	-5.63
0045eth	fluorobenzene	C <sub>7</sub> H <sub>6</sub> O	-3.45	-4.94
0062dio	fluorobenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.18	-5.36
0076but	fluorobenzene	C <sub>4</sub> H <sub>8</sub> O	-4.60	-5.23
0157flu	fluorobenzene	C <sub>6</sub> H <sub>5</sub> F	-4.60	-5.49
0506nit	fluorobenzene	CH <sub>3</sub> NO <sub>2</sub>	-4.62	-5.50
0008noc	chlorobenzene	C <sub>6</sub> H <sub>18</sub>	-5.16	-5.07
0036tol	chlorobenzene	C <sub>7</sub> H <sub>8</sub>	-5.18	-5.52
0044met	chlorobenzene	CH <sub>4</sub> O	-2.44	-3.26
0045eth	chlorobenzene	C <sub>2</sub> H <sub>6</sub> O	-3.30	-4.03
0047pro	chlorobenzene	C <sub>3</sub> H <sub>8</sub> O	-3.82	-4.73
0049but	chlorobenzene	C <sub>4</sub> H <sub>10</sub> O	-4.31	-5.52
0052pen	chlorobenzene	C <sub>5</sub> H <sub>12</sub> O	-5.25	-6.19
0053phe	chlorobenzene	C <sub>6</sub> H <sub>6</sub> O	-6.96	-7.49
0054hex	chlorobenzene	C <sub>6</sub> H <sub>14</sub> O	-5.98	-6.95
0055ocr	chlorobenzene	C <sub>7</sub> H <sub>8</sub> O	-7.33	-8.30
0057pcr	chlorobenzene	C <sub>7</sub> H <sub>8</sub> O	-7.23	-8.30
0058hep	chlorobenzene	C <sub>7</sub> H <sub>16</sub> O	-6.78	-7.71
0062dio	chlorobenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.08	-5.09
0075pro	chlorobenzene	C <sub>3</sub> H <sub>6</sub> O	-3.86	-4.13
0076but	chlorobenzene	C <sub>4</sub> H <sub>8</sub> O	-4.47	-4.76
0078pen	chlorobenzene	C <sub>5</sub> H <sub>10</sub> O	-5.29	-5.40
0080hex	chlorobenzene	C <sub>6</sub> H <sub>12</sub> O	-5.84	-6.15
0081dim	chlorobenzene	C <sub>6</sub> H <sub>12</sub> O	-5.25	-5.35
0082hep	chlorobenzene	C <sub>7</sub> H <sub>14</sub> O	-6.46	-6.87
0087pro	chlorobenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.38	-6.08
0093met	chlorobenzene	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-4.00	-4.53
0094met	chlorobenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.55	-4.74
0095eth	chlorobenzene	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.63	-4.87
0097pro	chlorobenzene	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-5.15	-5.38
0098met	chlorobenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.83	-6.01
0099but	chlorobenzene	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.74	-6.01
0101pen	chlorobenzene	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	-6.49	-6.72
0103eth	chlorobenzene	C <sub>2</sub> H <sub>7</sub> N	-2.73	-3.29
0104dim	chlorobenzene	C <sub>2</sub> H <sub>7</sub> N	-2.75	-3.41
0106pro	chlorobenzene	C <sub>3</sub> H <sub>9</sub> N	-3.59	-4.01
0107tri	chlorobenzene	C <sub>3</sub> H <sub>9</sub> N	-2.82	-3.16
0118ani	chlorobenzene	C <sub>6</sub> H <sub>7</sub> N	-6.72	-7.65
0174chl	chlorobenzene	C <sub>6</sub> H <sub>5</sub> Cl	-5.66	-6.14
0215pbr	chlorobenzene	C <sub>6</sub> H <sub>5</sub> OBr	-8.54	-9.77
0216amm	chlorobenzene	H <sub>3</sub> N	-1.22	-2.40
0228met	chlorobenzene	CH <sub>3</sub> N	-2.16	-2.81
0506nit	chlorobenzene	CH <sub>3</sub> NO <sub>2</sub>	-4.32	-5.17
n011	chlorobenzene	C <sub>7</sub> H <sub>9</sub> N	-7.54	-8.33
0075pro	chlorohexane	C <sub>3</sub> H <sub>6</sub> O	-3.45	-3.41
0076but	chlorohexane	C <sub>4</sub> H <sub>8</sub> O	-4.10	-4.31
0078pen	chlorohexane	C <sub>5</sub> H <sub>10</sub> O	-4.84	-5.11
0080hex	chlorohexane	C <sub>6</sub> H <sub>12</sub> O	-5.42	-5.84
0081dim	chlorohexane	C <sub>6</sub> H <sub>12</sub> O	-4.98	-4.72
0093met	chlorohexane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-3.66	-3.58
0094met	chlorohexane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.20	-4.18
0095eth	chlorohexane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.25	-4.16
0097pro	chlorohexane	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-4.84	-4.79
0098met	chlorohexane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.41	-5.67
0099but	chlorohexane	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-5.37	-5.48
0008noc	ethyl acetate	C <sub>8</sub> H <sub>18</sub>	-4.72	-4.81
0036tol	ethyl acetate	C <sub>7</sub> H <sub>8</sub>	-5.05	-4.94
0044met	ethyl acetate	CH <sub>4</sub> O	-3.37	-3.67
0045eth	ethyl acetate	C <sub>2</sub> H <sub>6</sub> O	-4.24	-4.34
0046eth	ethyl acetate	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	-6.82	-6.17
0047pro	ethyl acetate	C <sub>3</sub> H <sub>8</sub> O	-4.90	-5.09
0049but	ethyl acetate	C <sub>4</sub> H <sub>10</sub> O	-5.77	-5.79
0052pen	ethyl acetate	C <sub>5</sub> H <sub>12</sub> O	-6.13	-6.40
0053phe	ethyl acetate	C <sub>6</sub> H <sub>6</sub> O	-8.70	-8.03
0054hex	ethyl acetate	C <sub>6</sub> H <sub>14</sub> O	-6.92	-7.07
0058hep	ethyl acetate	C <sub>7</sub> H <sub>16</sub> O	-7.56	-7.71
0062dio	ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.03	-4.67
0086eth	ethyl acetate	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-6.46	-5.99
0087pro	ethyl acetate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-6.95	-6.70
0088but	ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-7.34	-7.20
0095eth	ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.46	-4.54
0217wat	ethyl acetate	H <sub>2</sub> O	-4.26	-4.53
0236oct	ethyl acetate	C <sub>8</sub> H <sub>18</sub> O	-8.41	-8.36
0506nit	ethyl acetate	CH <sub>3</sub> NO <sub>2</sub>	-5.06	-4.56
n011	ethyl acetate	C <sub>7</sub> H <sub>9</sub> N	-7.63	-8.67
n191	ethyl acetate	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	-15.43	-10.42
n200	ethyl acetate	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> F	-16.10	-11.67

n203	ethyl acetate	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> Br	-17.93	-11.32
0008noc	acetic acid	C <sub>8</sub> H <sub>18</sub>	-3.93	-4.54
0036tol	acetic acid	C <sub>7</sub> H <sub>8</sub>	-4.53	-4.90
0045eth	acetic acid	C <sub>2</sub> H <sub>6</sub> O	-5.25	-4.03
0062dio	acetic acid	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.80	-4.40
0076but	acetic acid	C <sub>4</sub> H <sub>8</sub> O	-4.80	-3.95
0086eth	acetic acid	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-5.30	-5.53
0506nit	acetic acid	CH <sub>3</sub> NO <sub>2</sub>	-4.88	-4.13
0008noc	aniline	C <sub>8</sub> H <sub>18</sub>	-3.48	-4.64
0036tol	aniline	C <sub>7</sub> H <sub>8</sub>	-4.57	-4.87
0045eth	aniline	C <sub>2</sub> H <sub>6</sub> O	-4.45	-4.42
0062dio	aniline	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.65	-4.89
0076but	aniline	C <sub>4</sub> H <sub>8</sub> O	-4.87	-4.14
0086eth	aniline	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-6.30	-6.03
0087pro	aniline	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-6.20	-6.29
0118ani	aniline	C <sub>6</sub> H <sub>7</sub> N	-7.61	-8.41
0506nit	aniline	CH <sub>3</sub> NO <sub>2</sub>	-5.11	-4.52
0008noc	dimethylpyridine	C <sub>8</sub> H <sub>18</sub>	-4.88	-4.82
0036tol	dimethylpyridine	C <sub>7</sub> H <sub>8</sub>	-5.03	-5.13
0045eth	dimethylpyridine	C <sub>2</sub> H <sub>6</sub> O	-4.87	-4.55
0062dio	dimethylpyridine	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-4.90	-4.73
0076but	dimethylpyridine	C <sub>4</sub> H <sub>8</sub> O	-4.34	-4.47
0125dim	dimethylpyridine	C <sub>7</sub> H <sub>9</sub> N	-6.04	-7.31
0008noc	tetrahydrofuran	C <sub>8</sub> H <sub>18</sub>	-5.39	-5.01
0036tol	tetrahydrofuran	C <sub>7</sub> H <sub>8</sub>	-5.50	-5.36
0045eth	tetrahydrofuran	C <sub>2</sub> H <sub>6</sub> O	-4.56	-4.83
0061tet	tetrahydrofuran	C <sub>4</sub> H <sub>8</sub> O	-4.25	-3.89
0062dio	tetrahydrofuran	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.17	-4.81
0076but	tetrahydrofuran	C <sub>4</sub> H <sub>8</sub> O	-4.54	-4.60
0506nit	tetrahydrofuran	CH <sub>3</sub> NO <sub>2</sub>	-5.09	-4.75
0053phe	decanol	C <sub>6</sub> H <sub>6</sub> O	-8.58	-7.41
0055ocr	decanol	C <sub>7</sub> H <sub>8</sub> O	-8.58	-8.01
0056mcr	decanol	C <sub>7</sub> H <sub>8</sub> O	-8.01	-8.07
0057pcr	decanol	C <sub>7</sub> H <sub>8</sub> O	-8.91	-8.12
0059dec	decanol	C <sub>10</sub> H <sub>22</sub> O	-9.58	-9.85
0103eth	decanol	C <sub>2</sub> H <sub>7</sub> N	-3.91	-3.54
0106pro	decanol	C <sub>3</sub> H <sub>9</sub> N	-4.59	-4.15
0110but	decanol	C <sub>4</sub> H <sub>11</sub> N	-5.22	-4.78
0146met	decanol	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	-5.41	-5.08
0174chl	decanol	C <sub>6</sub> H <sub>5</sub> Cl	-4.83	-5.16
0215pbr	decanol	C <sub>6</sub> H <sub>5</sub> OBr	-10.32	-9.60
0044met	tributyl phosphate	CH <sub>3</sub> O	-4.16	-3.10
0045eth	tributyl phosphate	C <sub>2</sub> H <sub>6</sub> O	-4.57	-3.51
0047pro	tributyl phosphate	C <sub>3</sub> H <sub>8</sub> O	-5.42	-4.07
0049but	tributyl phosphate	C <sub>4</sub> H <sub>10</sub> O	-6.28	-4.64
0052pen	tributyl phosphate	C <sub>5</sub> H <sub>12</sub> O	-6.69	-5.30
0054hex	tributyl phosphate	C <sub>6</sub> H <sub>14</sub> O	-7.68	-5.95
0058hep	tributyl phosphate	C <sub>7</sub> H <sub>16</sub> O	-7.98	-6.61
0086eth	tributyl phosphate	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-7.11	-4.41
0087pro	tributyl phosphate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-7.73	-4.69
0088but	tributyl phosphate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-8.29	-5.14
0089pen	tributyl phosphate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-8.82	-5.74
0103eth	tributyl phosphate	C <sub>2</sub> H <sub>7</sub> N	-3.29	-3.63
0106pro	tributyl phosphate	C <sub>3</sub> H <sub>9</sub> N	-3.98	-4.09
0118ani	tributyl phosphate	C <sub>6</sub> H <sub>7</sub> N	-7.60	-7.29
0146met	tributyl phosphate	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	-6.14	-4.83
0217wat	tributyl phosphate	H <sub>2</sub> O	-4.69	-4.57
0035ben	nonanol	C <sub>6</sub> H <sub>6</sub>	-3.82	-3.68
0036tol	nonanol	C <sub>7</sub> H <sub>8</sub>	-4.34	-4.34
0037eth	nonanol	C <sub>8</sub> H <sub>10</sub>	-4.61	-5.15
0053phe	nonanol	C <sub>6</sub> H <sub>6</sub> O	-8.61	-7.58
0103eth	nonanol	C <sub>2</sub> H <sub>7</sub> N	-4.02	-3.64
0106pro	nonanol	C <sub>3</sub> H <sub>9</sub> N	-4.66	-4.24
0110but	nonanol	C <sub>4</sub> H <sub>11</sub> N	-5.35	-4.87
0146met	nonanol	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	-5.61	-5.21
0215pbr	nonanol	C <sub>6</sub> H <sub>5</sub> OBr	-10.36	-9.76
0518non	nonanol	C <sub>9</sub> H <sub>20</sub> O	-9.05	-9.26
0008noc	dichloromethane	C <sub>8</sub> H <sub>18</sub>	-5.18	-5.06
0036tol	dichloromethane	C <sub>7</sub> H <sub>8</sub>	-5.53	-5.36
0045eth	dichloromethane	C <sub>2</sub> H <sub>6</sub> O	-3.82	-4.21
0053phe	dichloromethane	C <sub>6</sub> H <sub>6</sub> O	-7.50	-7.44
0057pcr	dichloromethane	C <sub>7</sub> H <sub>8</sub> O	-7.71	-8.03
0062dio	dichloromethane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-5.33	-5.43
0139thi	dichloromethane	C <sub>6</sub> H <sub>5</sub> S	-7.11	-8.15
0161dic	dichloromethane	CH <sub>2</sub> Cl <sub>2</sub>	-3.80	-3.46
0215pbr	dichloromethane	C <sub>6</sub> H <sub>5</sub> OBr	-9.09	-9.55
0217wat	dichloromethane	H <sub>2</sub> O	-2.63	-3.88
0506nit	dichloromethane	CH <sub>3</sub> NO <sub>2</sub>	-5.05	-5.02

1543 data MSE= -0.08 MAE= 0.42 RMSE= 0.71

Slope = 0.864 Intercept = -0.73 R<sup>2</sup>=0.853