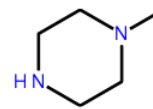


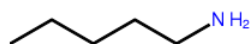
title: 1,4-dimethylpiperazine C<sub>6</sub>H<sub>14</sub>N<sub>2</sub>  
 Experimental: -7.58  
 Calculated SFE: -5.29



title: 1-Butanamine, ID: C109739  
 Experimental: -4.29  
 Calculated SFE: -2.52



title: 1-methylpiperazine C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>  
 Experimental: -7.77  
 Calculated SFE: -6.99



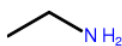
title: 1-pentanamine C<sub>5</sub>H<sub>13</sub>N  
 Experimental: -4.1  
 Calculated SFE: -2.41



title: 1-Propanamine, ID: C107108  
 Experimental: -4.39  
 Calculated SFE: -2.63



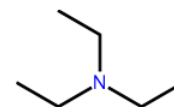
title: azetidine C<sub>3</sub>H<sub>7</sub>N  
 Experimental: -5.56  
 Calculated SFE: -3.45



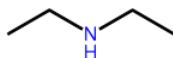
title: Ethylamine, ID: C75047  
 Experimental: -4.5  
 Calculated SFE: -2.94



title: Methylamine, ID: C74895  
 Experimental: -4.56  
 Calculated SFE: -2.98



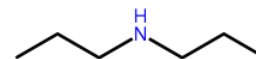
title: N,N-diethylethanamine C<sub>6</sub>H<sub>15</sub>N  
 Experimental: -4.07  
 Calculated SFE: -1.07



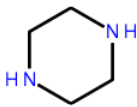
title: N-ethylethanamine C<sub>4</sub>H<sub>11</sub>N  
 Experimental: -4.5  
 Calculated SFE: -2.45



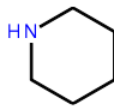
title: Methanamine, N-methyl-, ID: C124403  
 Experimental: -4.56  
 Calculated SFE: -2.47



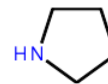
title: N-propylpropan-1-amine C<sub>6</sub>H<sub>15</sub>N  
 Experimental: -3.66  
 Calculated SFE: -1.83



title: piperazine C<sub>4</sub>H<sub>10</sub>N<sub>2</sub>  
Experimental: -7.4  
Calculated SFE: -7.63



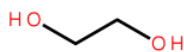
title: Piperidine, ID: C110894  
Experimental: -5.11  
Calculated SFE: -3.36



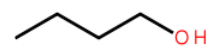
title: Pyrrolidine, ID: C123751  
Experimental: -5.48  
Calculated SFE: -3.71



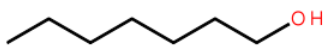
title: Trimethylamine, ID: C75503  
Experimental: -3.42  
Calculated SFE: -1.74



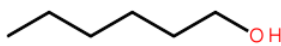
title: 1,2-Ethanediol, ID: C107211  
Experimental: -9.3  
Calculated SFE: -8.27



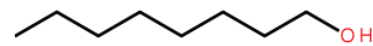
title: 1-Butanol, ID: C71363  
Experimental: -4.72  
Calculated SFE: -3.95



title: 1-Heptanol, ID: C111706  
Experimental: -4.42  
Calculated SFE: -3.26



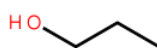
title: 1-Hexanol, ID: C111273  
Experimental: -4.36  
Calculated SFE: -3.39



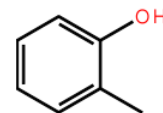
title: 1-Octanol, ID: C111875  
Experimental: -4.09  
Calculated SFE: -3.23



title: 1-Pentanol, ID: C71410  
Experimental: -4.47  
Calculated SFE: -3.59



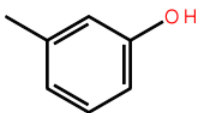
title: 1-Propanol, ID: C71238  
Experimental: -4.67  
Calculated SFE: -4.39



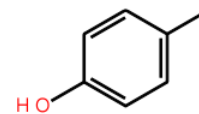
title: 2-methylphenol C<sub>7</sub>H<sub>8</sub>O  
Experimental: -5.87  
Calculated SFE: -4.73



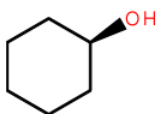
title: Isopropyl alcohol, ID: C67630  
Experimental: -4.76  
Calculated SFE: -4.15



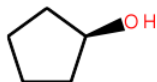
title: Phenol, 3-methyl-, ID: C108394  
Experimental: -5.49  
Calculated SFE: -5.18



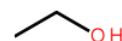
title: Phenol, 4-methyl-, ID: C106445  
Experimental: -6.14  
Calculated SFE: -5.4



title: Cyclohexanol, ID: C108930  
Experimental: -5.84  
Calculated SFE: -4.48



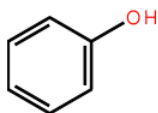
title: Cyclopentanol, ID: C96413  
Experimental: -5.49  
Calculated SFE: -4.72



title: Ethanol, ID: C64175  
Experimental: -5.01  
Calculated SFE: -4.45



title: Methyl alcohol, ID: C67561  
Experimental: -5.11  
Calculated SFE: -4.33



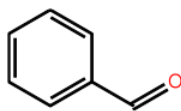
title: Phenol, ID: C108952  
Experimental: -6.62  
Calculated SFE: -4.64



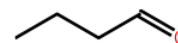
title: Ethanol, 1,1-dimethyl-, ID: C75650  
Experimental: -4.51  
Calculated SFE: -4.18



title: Acetaldehyde, ID: C75070  
Experimental: -3.5  
Calculated SFE: -2.1



title: Benzaldehyde, ID: C100527  
Experimental: -4.02  
Calculated SFE: -2.97



title: Butanal, ID: C123728  
Experimental: -3.18  
Calculated SFE: -1.8



title: Octanal, ID: C124130  
Experimental: -2.29  
Calculated SFE: -1.21



title: Pentanal, ID: C110623  
Experimental: -3.44  
Calculated SFE: -1.6



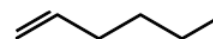
title: Propanal, ID: C123386  
Experimental: -3.44  
Calculated SFE: -2.11



title: 1,3-Butadiene, ID: C106990  
Experimental: 0.6  
Calculated SFE: 1.43



title: 1-Butene, ID: C106989  
Experimental: 1.38  
Calculated SFE: 2.25



title: 1-Hexene, ID: C592416  
Experimental: 1.68  
Calculated SFE: 2.83



title: 1-Pentene, ID: C109671  
Experimental: 1.66  
Calculated SFE: 2.42



title: 1-Propene, 2-methyl-, ID: C115117  
Experimental: 1.27  
Calculated SFE: 2.05



title: Cyclopentene, ID: C142290  
Experimental: 0.56  
Calculated SFE: 1.27



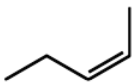
title: 2-Pentene, (E)-, ID: C646048  
Experimental: 1.34  
Calculated SFE: 2.3



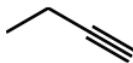
title: Ethylene, ID: C74851  
Experimental: 1.27  
Calculated SFE: 1.95



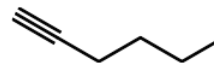
title: Propene, ID: C115071  
Experimental: 1.27  
Calculated SFE: 1.74



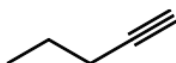
title: 2-Pentene, (Z)-, ID: C627203  
Experimental: 1.34  
Calculated SFE: 2.31



title: 1-Butyne, ID: C107006  
Experimental: -0.16  
Calculated SFE: 1.13



title: 1-Hexyne, ID: C693027  
Experimental: 0.29  
Calculated SFE: 1.58



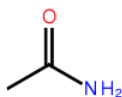
title: 1-Pentyne, ID: C627190  
Experimental: 0.01  
Calculated SFE: 1.19



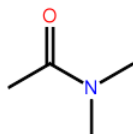
title: Acetylene, ID: C74862  
Experimental: -0.01  
Calculated SFE: 1.19



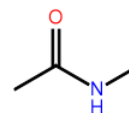
title: Propyne, ID: C74997  
Experimental: -0.31  
Calculated SFE: 0.97



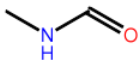
title: Acetamide, ID: C60355  
Experimental: -9.71  
Calculated SFE: -8.47



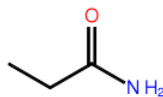
title: N,N-dimethylacetamide C4H9NO  
Experimental: -8.5  
Calculated SFE: -7.31



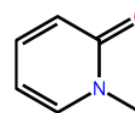
title: N-methylacetamide C3H7NO  
Experimental: -10.0  
Calculated SFE: -8.47



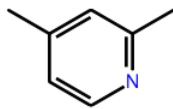
title: N-methylformamide C2H5NO  
Experimental: -10.0  
Calculated SFE: -6.63



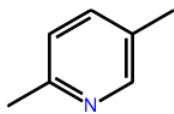
title: Propanamide, ID: C79050  
Experimental: -9.41  
Calculated SFE: -8.24



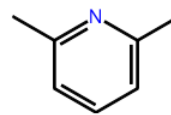
title: 1-methyl-1H-pyridin-2-one C6H7NO  
Experimental: -10.0  
Calculated SFE: -5.91



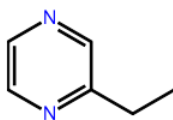
title: 2,4-dimethylpyridine C<sub>7</sub>H<sub>9</sub>N  
 Experimental: -4.86  
 Calculated SFE: -4.24



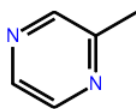
title: 2,5-dimethylpyridine C<sub>7</sub>H<sub>9</sub>N  
 Experimental: -4.72  
 Calculated SFE: -4.42



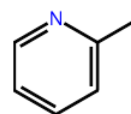
title: 2,6-dimethylpyridine C<sub>7</sub>H<sub>9</sub>N  
 Experimental: -4.6  
 Calculated SFE: -4.87



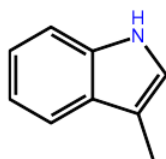
title: 2-ethylpyrazine C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>  
 Experimental: -5.51  
 Calculated SFE: -2.92



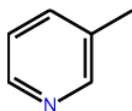
title: 2-methylpyrazine C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>  
 Experimental: -5.57  
 Calculated SFE: -3.33



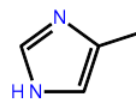
title: 2-methylpyridine C<sub>6</sub>H<sub>7</sub>N  
 Experimental: -4.63  
 Calculated SFE: -3.71



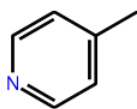
title: 3-methyl-1H-indole C<sub>9</sub>H<sub>9</sub>N  
 Experimental: -5.91  
 Calculated SFE: -4.73



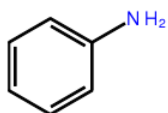
title: 3-methylpyridine C<sub>6</sub>H<sub>7</sub>N  
 Experimental: -4.77  
 Calculated SFE: -2.87



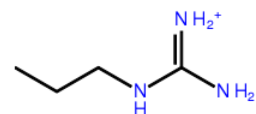
title: 4-methyl-1H-imidazole C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>  
 Experimental: -10.25  
 Calculated SFE: -8.5



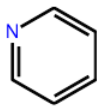
title: 4-methylpyridine C<sub>6</sub>H<sub>7</sub>N  
 Experimental: -4.94  
 Calculated SFE: -2.97



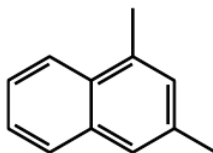
title: aniline C<sub>6</sub>H<sub>7</sub>N  
 Experimental: -5.5  
 Calculated SFE: -3.6



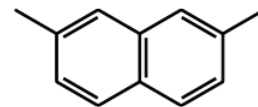
title: propylaminoformamidinium C<sub>4</sub>H<sub>11</sub>N<sub>3</sub>  
 Experimental: -10.92  
 Calculated SFE: -14.5



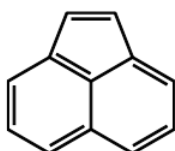
title: Pyridine, ID: C110861  
Experimental: -4.7  
Calculated SFE: -2.68



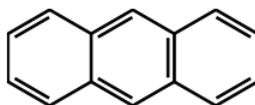
title: Naphthalene, 1,3-dimethyl-, ID: C575417  
Experimental: -2.47  
Calculated SFE: -2.36



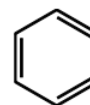
title: Naphthalene, 2,7-dimethyl-, ID: C582161  
Experimental: -2.63  
Calculated SFE: -2.45



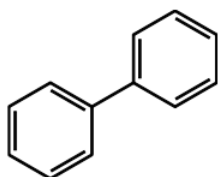
title: Acenaphthylene, ID: C208968  
Experimental: -3.15  
Calculated SFE: -2.11



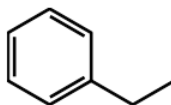
title: Anthracene, ID: C120127  
Experimental: -4.23  
Calculated SFE: -3.04



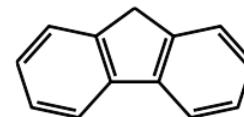
title: Benzene, ID: C71432  
Experimental: -0.87  
Calculated SFE: -0.06



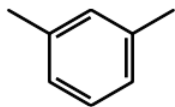
title: Biphenyl, ID: C92524  
Experimental: -2.64  
Calculated SFE: -1.4



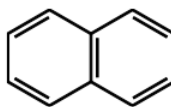
title: Ethylbenzene, ID: C100414  
Experimental: -0.8  
Calculated SFE: -0.46



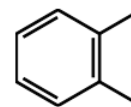
title: Fluorene, ID: C86737  
Experimental: -3.44  
Calculated SFE: -2.73



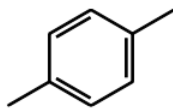
title: Benzene, 1,3-dimethyl-, ID: C108383  
Experimental: -0.84  
Calculated SFE: -1.06



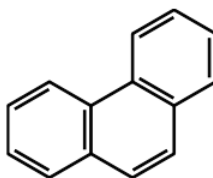
title: Naphthalene, ID: C91203  
Experimental: -2.29  
Calculated SFE: -1.63



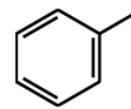
title: Benzene, 1,2-dimethyl-, ID: C95476  
Experimental: -0.9  
Calculated SFE: -1.54



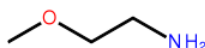
title: p-Xylene, ID: C106423  
 Experimental: -0.81  
 Calculated SFE: -1.33



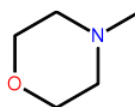
title: Phenanthrene, ID: C85018  
 Experimental: -3.95  
 Calculated SFE: -2.81



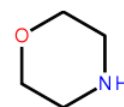
title: Toluene, ID: C108883  
 Experimental: -0.89  
 Calculated SFE: -0.74



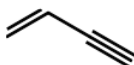
title: 2-methoxyethanamine C3H9NO  
 Experimental: -6.55  
 Calculated SFE: -4.84



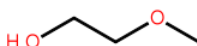
title: 4-methylmorpholine C5H11NO  
 Experimental: -6.34  
 Calculated SFE: -4.21



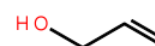
title: morpholine C4H9NO  
 Experimental: -7.17  
 Calculated SFE: -5.54



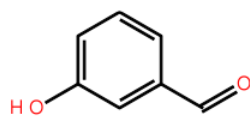
title: 1-Buten-3-yne, ID: C689974  
 Experimental: 0.04  
 Calculated SFE: 0.57



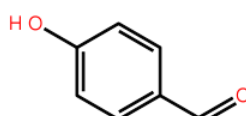
title: Ethanol, 2-methoxy-, ID: C109864  
 Experimental: -6.77  
 Calculated SFE: -4.95



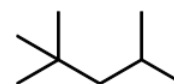
title: 2-Propen-1-ol, ID: C107186  
 Experimental: -5.08  
 Calculated SFE: -4.55



title: Benzaldehyde, 3-hydroxy-, ID: C100834  
 Experimental: -9.51  
 Calculated SFE: -7.94

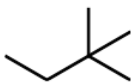


title: Benzaldehyde, 4-hydroxy-, ID: C123080  
 Experimental: -10.48  
 Calculated SFE: -7.9

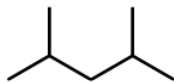


title: Pentane, 2,2,4-trimethyl-, ID: C540841  
 Experimental: 2.85  
 Calculated SFE: 2.87





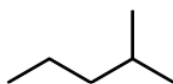
title: Butane, 2,2-dimethyl-, ID: C75832  
Experimental: 2.59  
Calculated SFE: 2.51



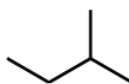
title: Pentane, 2,4-dimethyl-, ID: C108087  
Experimental: 2.88  
Calculated SFE: 2.95



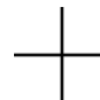
title: Isobutane, ID: C75285  
Experimental: 2.32  
Calculated SFE: 2.53



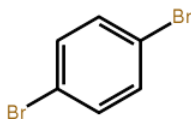
title: Pentane, 2-methyl-, ID: C107835  
Experimental: 2.52  
Calculated SFE: 2.92



title: Butane, 2-methyl-, ID: C78784  
Experimental: 2.38  
Calculated SFE: 2.63



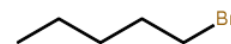
title: Propane, 2,2-dimethyl-, ID: C463821  
Experimental: 2.5  
Calculated SFE: 2.32



title: 1,4-dibromobenzene C<sub>6</sub>H<sub>4</sub>Br<sub>2</sub>  
Experimental: -2.3  
Calculated SFE: -1.6



title: 1-bromobutane C<sub>4</sub>H<sub>9</sub>Br  
Experimental: -0.41  
Calculated SFE: 0.08



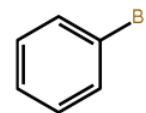
title: 1-bromopentane C<sub>5</sub>H<sub>11</sub>Br  
Experimental: -0.08  
Calculated SFE: 0.09



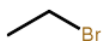
title: 1-bromopropane C<sub>3</sub>H<sub>7</sub>Br  
Experimental: -0.56  
Calculated SFE: -0.24



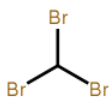
title: 2-bromopropane C<sub>3</sub>H<sub>7</sub>Br  
Experimental: -0.48  
Calculated SFE: -0.36



title: bromobenzene C<sub>6</sub>H<sub>5</sub>Br  
Experimental: -1.46  
Calculated SFE: -0.34



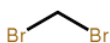
title: bromoethane C2H5Br  
Experimental: -0.7  
Calculated SFE: -0.4



title: bromoform CHBr3  
Experimental: -1.98  
Calculated SFE: -0.86



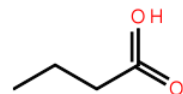
title: bromomethane CH3Br  
Experimental: -0.82  
Calculated SFE: -0.68



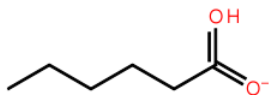
title: dibromomethane CH2Br2  
Experimental: -2.11  
Calculated SFE: -1.1



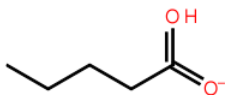
title: Acetic acid, ID: C64197  
Experimental: -6.7  
Calculated SFE: -5.44



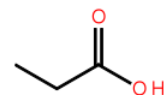
title: Butanoic acid, ID: C107926  
Experimental: -6.36  
Calculated SFE: -5.32



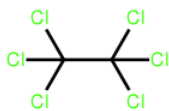
title: Hexanoic acid, ID: C142621  
Experimental: -6.21  
Calculated SFE: -4.49



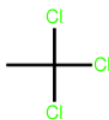
title: Pentanoic acid, ID: C109524  
Experimental: -6.16  
Calculated SFE: -5.06



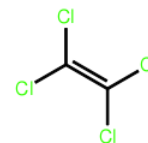
title: propionic C3H6O2  
Experimental: -6.47  
Calculated SFE: -5.31



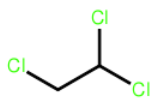
title: 1,1,1,2,2,2-hexachloroethane C2Cl6  
Experimental: 1.23  
Calculated SFE: 0.92



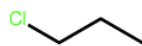
title: Ethane, 1,1,1-trichloro-, ID: C71556  
Experimental: -0.25  
Calculated SFE: 0.97



title: Tetrachloroethylene, ID: C127184  
Experimental: 0.05  
Calculated SFE: 0.85



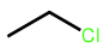
title: 1,1,2-trichloroethane C2H3Cl3  
Experimental: -1.95  
Calculated SFE: 0.45



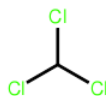
title: Propane, 1-chloro-, ID: C540545  
Experimental: -0.27  
Calculated SFE: 0.96



title: Propane, 2-chloro-, ID: C75296  
Experimental: -0.25  
Calculated SFE: 1.02



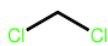
title: Ethyl chloride, ID: C75003  
Experimental: -0.63  
Calculated SFE: 0.56



title: Chloroform, ID: C67663  
Experimental: -1.07  
Calculated SFE: 0.2



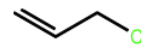
title: Methyl chloride, ID: C74873  
Experimental: -0.56  
Calculated SFE: 0.23



title: Methylene chloride, ID: C75092  
Experimental: -1.36  
Calculated SFE: -0.37



title: Carbon tetrachloride, ID: C56235  
Experimental: 0.1  
Calculated SFE: 0.25



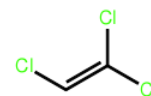
title: 3-chloroprop-1-ene C3H5Cl  
Experimental: -0.57  
Calculated SFE: 0.37



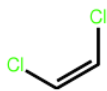
title: Ethene, chloro-, ID: C75014  
Experimental: -0.59  
Calculated SFE: 1.2



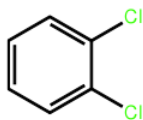
title: Ethene, 1,2-dichloro-, (E)-, ID: C156605  
Experimental: -0.76  
Calculated SFE: 0.68



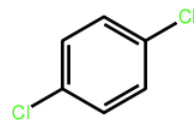
title: Trichloroethylene, ID: C79016  
Experimental: -0.39  
Calculated SFE: 0.29



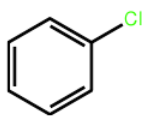
title: Ethene, 1,2-dichloro-, (Z)-, ID: C156592  
 Experimental: -1.17  
 Calculated SFE: -0.12



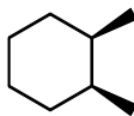
title: 1,2-dichlorobenzene C6H4Cl2  
 Experimental: -1.36  
 Calculated SFE: -0.64



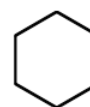
title: 1,4-dichlorobenzene C6H4Cl2  
 Experimental: -1.01  
 Calculated SFE: -0.63



title: chlorobenzene C6H5Cl  
 Experimental: -1.12  
 Calculated SFE: 0.29



title: Cyclohexane, 1,2-dimethyl-, cis-, ID: C2...  
 Experimental: 1.58  
 Calculated SFE: 1.71



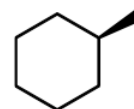
title: Cyclohexane, ID: C110827  
 Experimental: 1.23  
 Calculated SFE: 1.64



title: Cyclopentane, ID: C287923  
 Experimental: 1.2  
 Calculated SFE: 1.93



title: Cyclopropane, ID: C75194  
 Experimental: 0.75  
 Calculated SFE: 2.18



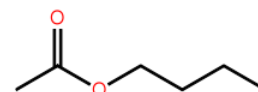
title: Cyclohexane, methyl-, ID: C108872  
 Experimental: 1.71  
 Calculated SFE: 1.65



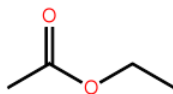
title: diethyldisulfide C4H10S2  
 Experimental: -1.43  
 Calculated SFE: -1.28



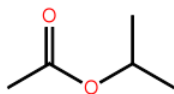
title: Disulfide, dimethyl, ID: C624920  
 Experimental: -1.54  
 Calculated SFE: -1.8



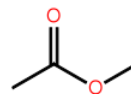
title: Acetic acid, butyl ester, ID: C123864  
 Experimental: -2.55  
 Calculated SFE: -1.05



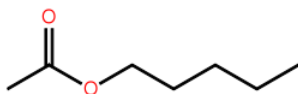
title: Ethyl acetate, ID: C141786  
Experimental: -3.1  
Calculated SFE: -3.47



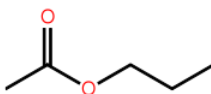
title: Acetic acid, 1-methylethyl ester, ID: C1...  
Experimental: -2.65  
Calculated SFE: -0.99



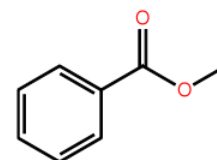
title: Acetic acid, methyl ester, ID: C79209  
Experimental: -3.32  
Calculated SFE: -1.54



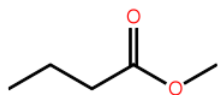
title: acetic acid pentyl ester C7H14O2  
Experimental: -2.45  
Calculated SFE: -0.5



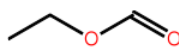
title: n-Propyl acetate, ID: C109604  
Experimental: -2.86  
Calculated SFE: -1.04



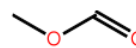
title: benzoic acid methyl ester C8H8O2  
Experimental: -4.28  
Calculated SFE: -2.44



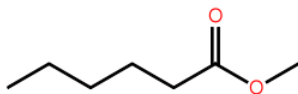
title: butyric acid methyl ester C5H10O2  
Experimental: -2.55  
Calculated SFE: -0.92



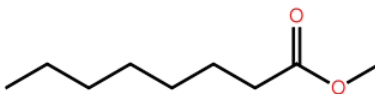
title: Formic acid, ethyl ester, ID: C109944  
Experimental: -2.65  
Calculated SFE: -1.07



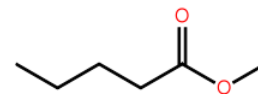
title: formic acid methyl ester C2H4O2  
Experimental: -2.78  
Calculated SFE: -3.46



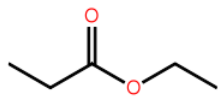
title: Hexanoic acid, methyl ester, ID: C106707  
Experimental: -2.49  
Calculated SFE: -0.55



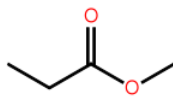
title: Octanoic acid, methyl ester, ID: C111115  
Experimental: -2.04  
Calculated SFE: -0.1



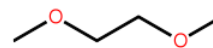
title: pentanoic acid methyl ester C6H12O2  
Experimental: -2.57  
Calculated SFE: -0.73



title: Propanoic acid, ethyl ester, ID: C105373  
 Experimental: -2.8  
 Calculated SFE: -1.07



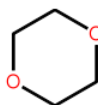
title: propionic acid ethyl ester C4H8O2  
 Experimental: -2.93  
 Calculated SFE: -1.21



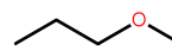
title: Ethane, 1,2-dimethoxy-, ID: C110714  
 Experimental: -3.86  
 Calculated SFE: -3.06



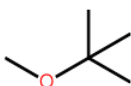
title: 1,3-Dioxolane, ID: C646060  
 Experimental: -4.1  
 Calculated SFE: -2.5



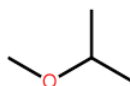
title: 1,4-Dioxane, ID: C123911  
 Experimental: -6.69  
 Calculated SFE: -2.6



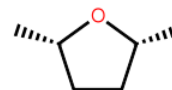
title: Methyl propyl ether, ID: C557175  
 Experimental: -1.59  
 Calculated SFE: -0.34



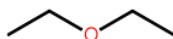
title: Propane, 2-methoxy-2-methyl-, ID: C1634044  
 Experimental: -0.79  
 Calculated SFE: -0.44



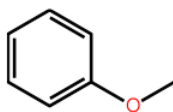
title: Propane, 2-methoxy-, ID: C598538  
 Experimental: -1.31  
 Calculated SFE: -0.46



title: cis-2,5-dimethyltetrahydrofuran C6H12O  
 Experimental: -2.92  
 Calculated SFE: -1.14



title: Ethoxy ethane, ID: C60297  
 Experimental: -2.64  
 Calculated SFE: -0.48



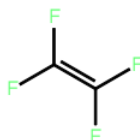
title: Benzene, methoxy-, ID: C100663  
 Experimental: -3.73  
 Calculated SFE: -0.72



title: Dimethyl ether, ID: C115106  
 Experimental: -2.64  
 Calculated SFE: -0.75



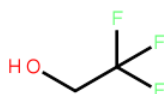
title: Furan, tetrahydro-, ID: C109999  
 Experimental: -3.84  
 Calculated SFE: -1.47



title: Ethene, tetrafluoro-, ID: C116143  
 Experimental: 1.38  
 Calculated SFE: 2.76



title: Ethane, 1,1-difluoro-, ID: C75376  
 Experimental: -0.11  
 Calculated SFE: 1.29



title: 2,2,2-trifluoroethanol C2H3F3O  
 Experimental: -4.31  
 Calculated SFE: -3.81



title: Methane, trifluoro-, ID: C75467  
 Experimental: 0.81  
 Calculated SFE: 1.64



title: Methyl fluoride, ID: C593533  
 Experimental: 0.73  
 Calculated SFE: 0.47



title: Carbon tetrafluoride, ID: C75730  
 Experimental: 3.11  
 Calculated SFE: 4.57



title: 1-iodobutane C4H9I  
 Experimental: -0.25  
 Calculated SFE: 0.19



title: 1-iodopentane C5H11I  
 Experimental: -0.12  
 Calculated SFE: 0.43



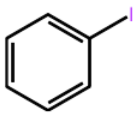
title: 1-iodopropane C3H7I  
 Experimental: -0.59  
 Calculated SFE: 0.14



title: 2-iodopropane C3H7I  
 Experimental: -0.46  
 Calculated SFE: 0.15



title: diiodomethane CH2I2  
 Experimental: -2.49  
 Calculated SFE: -2.27



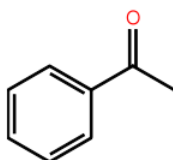
title: iodobenzene C<sub>6</sub>H<sub>5</sub>I  
Experimental: -1.73  
Calculated SFE: -0.59



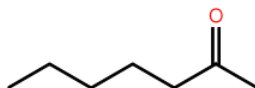
title: iodoethane C<sub>2</sub>H<sub>5</sub>I  
Experimental: -0.72  
Calculated SFE: 0.1



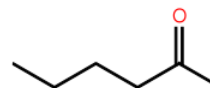
title: iodomethane CH<sub>3</sub>I  
Experimental: -0.89  
Calculated SFE: -0.36



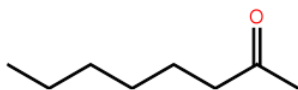
title: 1-phenylethanone C<sub>8</sub>H<sub>8</sub>O  
Experimental: -4.58  
Calculated SFE: -3.44



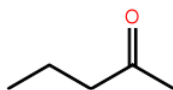
title: 2-Heptanone, ID: C110430  
Experimental: -3.04  
Calculated SFE: -1.92



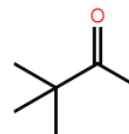
title: 2-hexanone C<sub>6</sub>H<sub>12</sub>O  
Experimental: -3.29  
Calculated SFE: -1.9



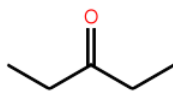
title: 2-Octanone, ID: C111137  
Experimental: -2.88  
Calculated SFE: -1.64



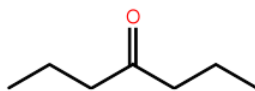
title: 2-Pentanone, ID: C107879  
Experimental: -3.41  
Calculated SFE: -2.47



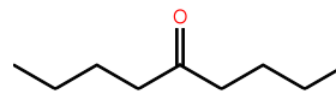
title: 3,3-dimethylbutan-2-one C<sub>6</sub>H<sub>12</sub>O  
Experimental: -2.89  
Calculated SFE: -2.05



title: 3-Pentanone, ID: C96220  
Experimental: -3.41  
Calculated SFE: -2.48



title: 4-Heptanone, ID: C123193  
Experimental: -2.93  
Calculated SFE: -2.38

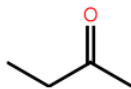


title: 5-nonanone C<sub>9</sub>H<sub>18</sub>O  
Experimental: -2.67  
Calculated SFE: -1.75

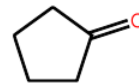




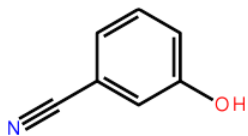
title: Acetone, ID: C67641  
Experimental: -3.85  
Calculated SFE: -2.64



title: 2-Butanone, ID: C78933  
Experimental: -3.64  
Calculated SFE: -2.31



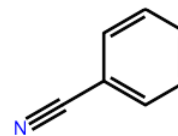
title: Cyclopentanone, ID: C120923  
Experimental: -4.68  
Calculated SFE: -3.05



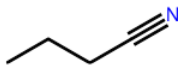
title: 3-hydroxybenzonitrile C7H5NO  
Experimental: -9.67  
Calculated SFE: -6.98



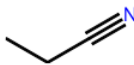
title: Acetonitrile, ID: C75058  
Experimental: -3.89  
Calculated SFE: -3.7



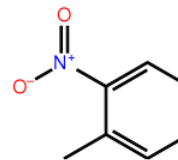
title: benzonitrile C7H5N  
Experimental: -4.1  
Calculated SFE: -2.3



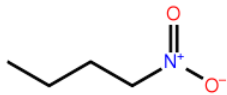
title: Butanenitrile, ID: C109740  
Experimental: -3.64  
Calculated SFE: -3.09



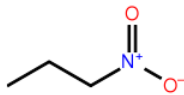
title: propionitrile C3H5N  
Experimental: -3.85  
Calculated SFE: -3.39



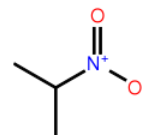
title: 1-methyl-2-nitro-benzene C7H7NO2  
Experimental: -3.59  
Calculated SFE: -2.55



title: 1-nitrobutane C4H9NO2  
Experimental: -3.08  
Calculated SFE: -2.63



title: 1-nitropropane C3H7NO2  
Experimental: -3.34  
Calculated SFE: -2.58



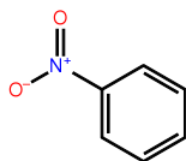
title: 2-nitropropane C3H7NO2  
Experimental: -3.14  
Calculated SFE: -2.3



title: 3-nitrophenol C<sub>6</sub>H<sub>5</sub>NO<sub>3</sub>

Experimental: -9.63

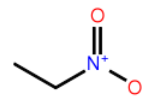
Calculated SFE: -7.61



title: nitrobenzene C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>

Experimental: -4.12

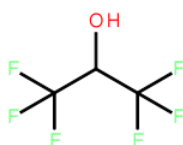
Calculated SFE: -2.61



title: nitroethane C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>

Experimental: -3.71

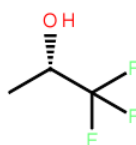
Calculated SFE: -2.75



title: 1,1,1,3,3,3-hexafluoropropan-2-ol C<sub>3</sub>H<sub>2</sub>F<sub>6</sub>O

Experimental: -3.77

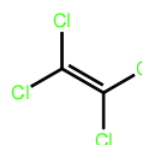
Calculated SFE: -2.08



title: 1,1,1-trifluoropropan-2-ol C<sub>3</sub>H<sub>5</sub>F<sub>3</sub>O

Experimental: -4.16

Calculated SFE: -3.13



title: 1,1,2,2-tetrachloroethylene C<sub>2</sub>Cl<sub>4</sub>

Experimental: 0.05

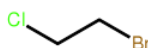
Calculated SFE: 0.76



title: 1,1,2-trichloro-1,2,2-trifluoro-ethane C<sub>2</sub>F<sub>3</sub>Cl<sub>3</sub>

Experimental: 1.77

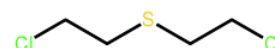
Calculated SFE: 1.56



title: 1-bromo-2-chloro-ethane C<sub>2</sub>H<sub>4</sub>BrCl

Experimental: -1.95

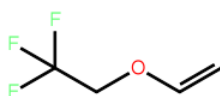
Calculated SFE: -1.15



title: 1-chloro-2-(2-chloroethylsulfanyl)ethane C<sub>4</sub>H<sub>8</sub>Cl<sub>2</sub>S

Experimental: -3.92

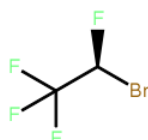
Calculated SFE: -2.31



title: 2,2,2-trifluoroethoxyethylene C<sub>4</sub>H<sub>5</sub>F<sub>3</sub>O

Experimental: -0.12

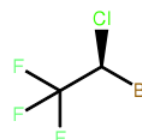
Calculated SFE: -0.01



title: 2-bromo-1,1,1,2-tetrafluoro-ethane C<sub>2</sub>HBrF<sub>4</sub>

Experimental: 0.52

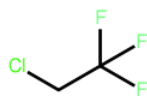
Calculated SFE: -1.29



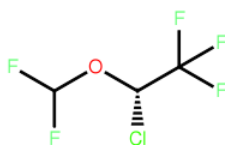
title: 2-bromo-2-chloro-1,1,1-trifluoro-ethane C<sub>2</sub>BrClF<sub>4</sub>

Experimental: -0.13

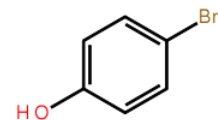
Calculated SFE: -0.59



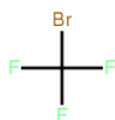
title: 2-chloro-1,1,1-trifluoro-ethane C<sub>2</sub>H<sub>2</sub>ClF<sub>3</sub>  
 Experimental: 0.06  
 Calculated SFE: 0.59



title: 2-chloro-2-(difluoromethoxy)-1,1,1-trifl...  
 Experimental: 0.11  
 Calculated SFE: 0.59



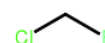
title: 4-bromophenol C<sub>6</sub>H<sub>5</sub>BrO  
 Experimental: -7.13  
 Calculated SFE: -5.56



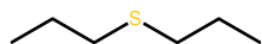
title: bromo-trifluoro-methane CBrF<sub>3</sub>  
 Experimental: 1.79  
 Calculated SFE: 0.53



title: chloro-difluoro-methane CHClF<sub>2</sub>  
 Experimental: -0.5  
 Calculated SFE: 0.81



title: chloro-fluoro-methane CH<sub>2</sub>ClF  
 Experimental: -0.77  
 Calculated SFE: 0.1



title: 1-propylsulfanylpropane C<sub>6</sub>H<sub>14</sub>S  
 Experimental: -1.27  
 Calculated SFE: 0.46



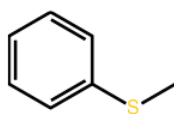
title: Diethyl sulfide, ID: C352932  
 Experimental: -1.43  
 Calculated SFE: -0.19



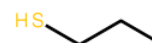
title: Dimethyl sulfide, ID: C75183  
 Experimental: -1.54  
 Calculated SFE: -0.62



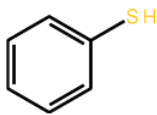
title: hydrogen sulfide H<sub>2</sub>S  
 Experimental: -0.7  
 Calculated SFE: 1.01



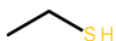
title: methylsulfanylbenzene C<sub>7</sub>H<sub>8</sub>S  
 Experimental: -2.73  
 Calculated SFE: -1.22



title: 1-Propanethiol, ID: C107039  
 Experimental: -1.05  
 Calculated SFE: -0.06



title: benzenethiol C6H6S  
Experimental: -2.55  
Calculated SFE: -0.75



title: Ethanethiol, ID: C75081  
Experimental: -1.3  
Calculated SFE: -0.29



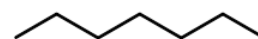
title: Methanethiol, ID: C74931  
Experimental: -1.24  
Calculated SFE: -0.51



title: Butane, ID: C106978  
Experimental: 2.08  
Calculated SFE: 2.54



title: Ethane, ID: C74840  
Experimental: 1.83  
Calculated SFE: 2.3



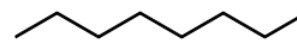
title: Heptane, ID: C142825  
Experimental: 2.62  
Calculated SFE: 2.88



title: Hexane, ID: C110543  
Experimental: 2.49  
Calculated SFE: 2.83



title: Methane, ID: C74828  
Experimental: 2.0  
Calculated SFE: 2.2



title: Octane, ID: C111659  
Experimental: 2.89  
Calculated SFE: 3.55



title: Pentane, ID: C109660  
Experimental: 2.33  
Calculated SFE: 2.48



title: Propane, ID: C74986  
Experimental: 1.96  
Calculated SFE: 2.42