

## **Classification Study of Solvation Free Energy of Organic Molecules with Machine Learning Techniques**

N.S. Hari Narayana Moorthy\*, Silvia A. Martins, Sergio F Sousa, Maria J. Ramos, Pedro A.  
Fernandes

REQUIMTE, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade  
do Porto, s/n, Rua do Campo Alegre, 4169-007 Porto, Portugal.

**Table S1: List of molecules considered for the classification analysis along with their solvation free energies**

<b>Molecular Code</b>	<b>Molecule name</b>	<b>Type of molecules</b>	<b>Solvation free energy (kcal/mol)</b>
DB0001	Methane	Alkane	1.97
DB0002	Ethane	Alkane	1.83
DB0003	Propane	Alkane	1.97
DB0004	Butane	Alkane	2.10
DB0005	Pentane	Alkane	2.33
DB0006	Hexane	Alkane	2.50
DB0007	Heptane	Alkane	2.64
DB0008	Octane	Alkane	2.89
DB0009	2-methylpropane	Alkane	2.31
DB0010	2-methylbutane	Alkane	2.38
DB0011	2-methylpentane	Alkane	2.52
DB0012	3-methylpentane	Alkane	2.51
DB0013	2-methylhexane	Alkane	2.93
DB0014	3-methylhexane	Alkane	2.71
DB0015	3-methylheptane	Alkane	2.97
DB0016	cyclopentane	Alkane	1.20
DB0017	cyclohexane	Alkane	1.23
DB0018	cycloheptane	Alkane	0.80
DB0019	cyclooctane	Alkane	0.86
DB0020	Benzene	Arenes	-0.87
DB0021	Toluene	Arenes	-0.83
DB0022	o-xylene	Arenes	-0.90
DB0023	m-xylene	Arenes	-0.82
DB0024	p-xylene	Arenes	-0.81
DB0025	naphtalene	Arenes	-2.41
DB0026	anthracene	Arenes	-4.17
DB0027	phenanthrene	Arenes	-3.99
DB0028	Pyridine	Heterocyclics	-4.69
DB0029	Pyrrole	Heterocyclics	-4.78
DB0030	Thiophene	Heterocyclics	-1.42
DB0031	Imidazole	Heterocyclics	-9.63
DB0032	Methanol	Alcohols and Phenols	-5.10
DB0033	Ethanol	Alcohols and Phenols	-4.96
DB0034	1-Propanol	Alcohols and Phenols	-4.85
DB0035	1-Butanol	Alcohols and Phenols	-4.73
DB0036	1-Pentanol	Alcohols and Phenols	-4.52
DB0037	1-Hexanol	Alcohols and Phenols	-4.38
DB0038	1-Heptanol	Alcohols and Phenols	-4.25
DB0039	1-Octanol	Alcohols and Phenols	-4.11
DB0040	2-Propanol	Alcohols and Phenols	-4.76
DB0041	2-Butanol	Alcohols and Phenols	-4.61
DB0042	2-Pentanol	Alcohols and Phenols	-4.40
DB0043	3-Pentanol	Alcohols and Phenols	-4.35
DB0044	3-Hexanol	Alcohols and Phenols	-3.91
DB0045	4-Heptanol	Alcohols and Phenols	-4.01

DB0046	2-methylpropane-2-ol	Alcohols and Phenols	-4.49
DB0047	2-methylbutane-2-ol	Alcohols and Phenols	-4.43
DB0048	2-methylpentane-2-ol	Alcohols and Phenols	-3.93
DB0049	Cyclopentanol	Alcohols and Phenols	-5.49
DB0050	Cyclohexanol	Alcohols and Phenols	-5.28
DB0051	Cycloheptanol	Alcohols and Phenols	-5.49
DB0052	Phenol	Alcohols and Phenols	-6.59
DB0053	2-methylphenol	Alcohols and Phenols	-5.87
DB0054	3-methylphenol	Alcohols and Phenols	-5.49
DB0055	4-methylphenol	Alcohols and Phenols	-6.13
DB0056	2,3-dimethylphenol	Alcohols and Phenols	-6.16
DB0057	3,4-dimethylphenol	Alcohols and Phenols	-6.50
DB0058	2,6-dimethylphenol	Alcohols and Phenols	-5.26
DB0059	2,4-dimethylphenol	Alcohols and Phenols	-6.01
DB0060	3,5-dimethylphenol	Alcohols and Phenols	-6.27
DB0061	2,5-dimethylphenol	Alcohols and Phenols	-5.91
DB0062	1-hydroxynapthalene	Alcohols and Phenols	-7.67
DB0063	2-hydroxynapthalene	Alcohols and Phenols	-8.11
DB0064	Nonane	Alkane	3.13
DB0065	2,2-dimethylpropane	Alkane	2.53
DB0066	2,2-dimethylbutane	Alkane	2.57
DB0067	2,2-dimethylpentane	Alkane	2.88
DB0068	3,3-dimethylpentane	Alkane	2.56
DB0069	Methylcyclopentane	Alkane	1.60
DB0070	Methylcyclohexane	Alkane	1.71
DB0071	1,2,3-trimethylbenzene	Arenes	-1.21
DB0072	1,2,4-trimethylbenzene	Arenes	-0.86
DB0073	1,3,5-trimethylbenzene	Arenes	-0.90
DB0074	1-Methylnapthalene	Arenes	-2.40
DB0075	1,3-Dimethylnapthalene	Arenes	-2.47
DB0076	1,4-Dimethylnapthalene	Arenes	-2.82
DB0077	2,3-Dimethylnapthalene	Arenes	-2.78
DB0078	2,6-Dimethylnapthalene	Arenes	-2.63
DB0079	2,7-Dimethylnapthalene	Arenes	-2.63
DB0080	2-methylpyridine	Heterocyclics	-4.63
DB0081	3-methylpyridine	Heterocyclics	-4.77
DB0082	4-methylpyridine	Heterocyclics	-4.91
DB0083	2,3-dimethylpyridine	Heterocyclics	-4.82
DB0084	2,4-dimethylpyridine	Heterocyclics	-4.86
DB0085	2,5-dimethylpyridine	Heterocyclics	-4.71
DB0086	2,6-dimethylpyridine	Heterocyclics	-4.60
DB0087	3,4-dimethylpyridine	Heterocyclics	-5.22
DB0088	3,5-dimethylpyridine	Heterocyclics	-4.84
DB0089	2-Methylindole	Heterocyclics	-5.90
DB0090	3-Methylindole	Heterocyclics	-5.88
DB0091	2-Methylthiophene	Heterocyclics	-1.38
DB0092	2-Methylimidazole	Heterocyclics	-10.25
DB0093	4-Methylimidazole	Heterocyclics	-10.27
DB0094	Chloroethane	Haloalkanes	-0.63
DB0095	Bromoethane	Haloalkanes	-0.71

DB0096	Iodoethane	Haloalkanes	-0.73
DB0097	1-chloropropane	Haloalkanes	-0.32
DB0098	Bromopropane	Haloalkanes	-0.56
DB0099	1-Iodopropane	Haloalkanes	-0.56
DB0100	1-Chlorobutane	Haloalkanes	-0.15
DB0101	1-Bromobutane	Haloalkanes	-0.41
DB0102	1-Iodobutane	Haloalkanes	-0.26
DB0103	1-Chloropentane	Haloalkanes	-0.07
DB0104	2-chloropropane	Haloalkanes	-0.25
DB0105	2-Bromopropane	Haloalkanes	-0.48
DB0106	2-Iodopropane	Haloalkanes	-0.46
DB0107	2-Chlorobutane	Haloalkanes	0.07
DB0108	2-Chloropentane	Haloalkanes	0.07
DB0109	3-Chloropentane	Haloalkanes	0.06
DB0110	2-chloro-2-methylpropane	Haloalkanes	1.09
DB0111	2-bromo-2-methylpropane	Haloalkanes	0.84
DB0112	Fluorobenzene	Halobenzene	-0.79
DB0113	Chlorobenzene	Halobenzene	-1.09
DB0114	Bromobenzene	Halobenzene	-1.46
DB0115	Iodobenzene	Halobenzene	-1.74
DB0116	2-Chlorotoluene	Halophenyl	-1.15
DB0117	2-Bromotoluene	Halophenyl	-2.37
DB0118	m-chlorotoluene	Halophenyl	-1.92
DB0119	p-chlorotoluene	Halophenyl	1.92
DB0120	p-bromotoluene	Halophenyl	-1.39
DB0121	1,1-difluoroethane	Haloalkanes	-0.11
DB0122	1,1 dichloroethane	Haloalkanes	-0.85
DB0123	1,2 dichloroethane	Haloalkanes	-1.79
DB0124	1,1,1 trichloroethane	Haloalkanes	-0.23
DB0125	1,1,2 trichloroethane	Haloalkanes	-1.97
DB0126	1,1,1,2 tetrachloroethane	Haloalkanes	-1.20
DB0127	1,1,2,2 tetrachloroethane	Haloalkanes	-2.42
DB0128	1,2-dibromoethane	Haloalkanes	-2.22
DB0129	1,2 dichloropropane	Haloalkanes	-1.26
DB0130	1,3 dichloropropane	Haloalkanes	-1.90
DB0131	1,2-dibromopropane	Haloalkanes	-1.94
DB0132	1,3-dibromopropane	Haloalkanes	-1.97
DB0133	1,1-dichlorobutane	Haloalkanes	-0.70
DB0134	1,4-dichlorobutane	Haloalkanes	-2.32
DB0135	1,2-dichlorobenzene	Halobenzene	-1.36
DB0136	1,3-dichlorobenzene	Halobenzene	-0.98
DB0137	1,4-dichlorobenzene	Halobenzene	-1.01
DB0138	1,4-dibromobenzene	Halobenzene	-2.30
DB0139	1,2,3-trichlorobenzene	Halobenzene	-1.24
DB0140	1,2,4-trichlorobenzene	Halobenzene	-1.12
DB0141	1,3,5-trichlorobenzene	Halobenzene	-0.78
DB0142	1,2,3,4-tetrachlorobenzene	Halobenzene	-1.34
DB0143	1,2,3,5-tetrachlorobenzene	Halobenzene	-1.62
DB0144	1,2,4,5-tetrachlorobenzene	Halobenzene	-1.34
DB0145	Methyl amine	Amines	-4.57

DB0146	Ethyl amine	Amines	-4.49
DB0147	n-propyl amine	Amines	-4.44
DB0148	n-butyl amine	Amines	-4.32
DB0149	n-pentyl amine	Amines	-4.10
DB0150	n-hexyl amine	Amines	-4.02
DB0151	n-heptylamine	Amines	-3.79
DB0152	n-octylamine	Amines	-3.65
DB0153	Ethylenediamine	Amines	-9.82
DB0154	cyclohexylamine	Amines	-4.59
DB0155	Aniline	Amines	-5.39
DB0156	Dimethyl amine	Amines	-4.30
DB0157	Diethyl amine	Amines	-4.08
DB0158	Di-n-propylamine	Amines	-3.67
DB0159	Di-n-butyl amine	Amines	-3.32
DB0160	Trimethyl amine	Amines	-3.23
DB0161	Pyrrolidine	Amines	-5.49
DB0162	Piperidine	Amines	-5.12
DB0163	N-Methylpyrrolidine	Amines	-3.99
DB0164	N-Methylpiperidine	Amines	-3.88
DB0165	Piperazine	Amines	-7.39
DB0166	N-methylpiperazine	Amines	-7.77
DB0167	Diisopropylamine	Amines	-3.22
DB0168	Triethyl amine	Amines	-3.09
DB0169	Aziridine		-5.42
DB0170	Azetidine		-5.56
DB0171	Morpholine		-7.17
DB0172	N-methylmorpholine		-6.33
DB0173	Ammonia		-4.30
DB0174	N,N-Dimethyl aniline	Amines	-2.90
DB0175	N,N-Dimethylpiperazine	Amines	-7.58
DB0176	1-Amino-2-methoxy-ethane	Amines	-6.60
DB0177	N-Methyl formamide	Amides	-10.00
DB0178	Acetamide	Amides	-9.71
DB0179	Propionamide	Amides	-9.42
DB0180	benzamide	Amides	-10.97
DB0181	N-Methylacetamide	Amides	-10.04
DB0182	N,N-Dimethylformamide	Amides	-7.81
DB0183	N,N-Dimethyl-acetamide	Amides	-8.53
DB0184	n-butylacetamide	Amides	-9.31
DB0185	nitromethane	Nitro compounds	-4.00
DB0186	nitroethane	Nitro compounds	-3.72
DB0187	1-nitropropane	Nitro compounds	-3.34
DB0188	1-nitrobutane	Nitro compounds	-3.08
DB0189	1-nitropentane	Nitro compounds	-2.82
DB0190	2-nitropropane	Nitro compounds	-3.14
DB0191	nitrobenzene	Nitro compounds	-4.13
DB0192	2-nitrophenol	Nitro compounds	-4.58
DB0193	3-nitrophenol	Nitro compounds	-9.63
DB0194	p-nitrophenol	Nitro compounds	-10.65

DB0195	2-nitrotoluene	Nitro compounds	-3.59
DB0196	3-nitrotoluene	Nitro compounds	-3.46
DB0197	m-nitroaniline	Nitro compounds	-8.86
DB0198	acetaldehyde	Aldehydes	-3.50
DB0199	propionaldehyde	Aldehydes	-3.43
DB0200	butyraldehyde	Aldehydes	-3.18
DB0201	Pentanal	Aldehydes	-3.03
DB0202	Hexanal	Aldehydes	-2.81
DB0203	Heptanal	Aldehydes	-2.67
DB0204	Octanal	Aldehydes	-2.29
DB0205	Nonanal	Aldehydes	-2.07
DB0206	isobutaldehyde	Aldehydes	-2.86
DB0207	Benzaldehyde	Aldehydes	-4.02
DB0208	m-Hydroxybenzaldehyde	Aldehydes	-9.51
DB0209	p-Hydroxybenzaldehyde	Aldehydes	-10.48
DB0210	formaldehyde	Aldehydes	-2.75
DB0211	Ethanoic acid	Carboxylic Acids	-6.69
DB0212	Propanoic acid	Carboxylic Acids	-6.46
DB0213	Butanoic acid	Carboxylic Acids	-6.35
DB0214	Pentanoic acid	Carboxylic Acids	-6.16
DB0215	Hexanoic acid	Carboxylic Acids	-6.21
DB0216	methoxymethane	Ethers	-1.91
DB0217	methyl-ethyl-ether	Ethers	-2.10
DB0218	Methyl propyl ether	Ethers	-1.66
DB0219	Methyl isopropyl ether	Ethers	-2.01
DB0220	t-Butyl methyl ether	Ethers	-2.21
DB0221	2-Methoxyethanol	Ethers	-6.76
DB0222	2-methoxyethanamine	Ethers	-6.55
DB0223	2-methoxyphenol	Ethers	-5.57
DB0224	3-methoxyphenol	Ethers	-7.66
DB0225	2-methoxyaniline	Ethers	-6.12
DB0226	3-methoxyaniline	Ethers	-7.29
DB0227	4-methoxyaniline	Ethers	-7.48
DB0228	Methanethiol	Thiols	-1.24
DB0229	Ethanethiol	Thiols	-1.19
DB0230	1-Propanethiol	Thiols	-1.06
DB0231	n-butanethiol	Thiols	-0.99
DB0232	Thiophenol	Thiols	-2.55
DB0233	acetonitrile	Nitriles	-3.89
DB0234	propanenitrile	Nitriles	-3.85
DB0235	butanenitrile	Nitriles	-3.65
DB0236	pentanenitrile	Nitriles	-3.52
DB0237	benzonitrile	Nitriles	-4.16
DB0238	3-cyanophenol	Nitriles	-9.66
DB0239	4-cyanophenol	Nitriles	-10.17
DB0240	3-cyanopyridine	Nitriles	-6.75
DB0241	4-cyanopyridine	Nitriles	-6.02