DB num.	Name	Solvation Free Energy (kJ/mol)		
		Water	Cyclohexane	Octanol
159	methanol	-14.56 ± 0.05	-3.7 ± 0.1	-12.9 ± 0.2
492	acetone	-14.9 ± 0.1	-10.0 ± 0.1	-16.0 ± 0.2
671	trimethylamine	-11.2 ± 0.1	-12.1 ± 0.1	-17.4 ± 0.2
835	2-2-2-trichloro-1-dimethoxyphosphorylethanol	-55.7 ± 0.1	-42.5 ± 0.1	-68.6 ± 0.5
950	butanol	-13.5 ± 0.1	-14.4 ± 0.1	-22.5 ± 0.2
1014	butylamine	-12.6 ± 0.1	-15.1 ± 0.1	-19.6 ± 0.2
1028	diethylamine	-12.5 ± 0.1	-15.2 ± 0.1	-20.7 ± 0.2
1307	pentachlorophenol	-14.6 ± 0.1	-43.5 ± 0.1	-51.9 ± 0.3
1363	quinone	-29.1 ± 0.1	-23.7 ± 0.1	-32.6 ± 0.3
1425	p-iodophenol	-24.9 ± 0.1	-30.0 ± 0.1	-45.1 ± 0.2
1453	o-nitrophenol	-22.7 ± 0.1	-33.6 ± 0.1	-37.5 ± 0.3
1711	aniline	-23.0 ± 0.1	-19.8 ± 0.1	-26.6 ± 0.2
1879	nitrocyclohexane	-9.8 ± 0.1	-31.8 ± 0.1	-32.3 ± 0.2
2133	benzaldehyde	-21.2 ± 0.1	-21.7 ± 0.1	-29.5 ± 0.2
2185	salicylic acid	-27.7 ± 0.2	-31.5 ± 0.1	-41.0 ± 0.2
2323	m-methylphenol	-22.7 ± 0.1	-22.2 ± 0.1	-33.0 ± 0.2
2336	o-methylphenol	-21.0 ± 0.1	-22.0 ± 0.1	-31.8 ± 0.3
2348	p-methylphenol	-23.2 ± 0.1	-22.4 ± 0.1	-34.5 ± 0.2
2411	o-toluidine	-22.6 ± 0.1	-22.8 ± 0.1	-28.9 ± 0.2
2422	p-toluidine	-22.7 ± 0.1	-22.9 ± 0.1	-29.9 ± 0.2
2612	phthalimide	-50.0 ± 0.1	-36.3 ± 0.1	-57.8 ± 0.4
2790	vanillin	-33.8 ± 0.1	-33.3 ± 0.1	-43.5 ± 0.3
2914	2-4-dimethylphenol	-20.5 ± 0.1	-25.6 ± 0.1	-34.0 ± 0.2
2917	2-5-dimethylphenol	-20.8 ± 0.1	-25.1 ± 0.1	-33.8 ± 0.3
2925	3-4-dimethylphenol	-22.8 ± 0.1	-25.6 ± 0.1	-36.6 ± 0.2
2938	p-ethylphenol	-22.6 ± 0.1	-25.4 ± 0.1	-36.1 ± 0.2
3110	5-cyano-2-(trifluoromethyl)-1h-benzimidazole	-45.5 ± 0.1	-44.0 ± 0.1	-69.8 ± 0.3
3126	coumarin	-34.2 ± 0.1	-33.3 ± 0.1	-47.9 ± 0.3
3130	1-3-indanedione	-31.8 ± 0.1	-33.3 ± 0.1	-42.2 ± 0.3
3228	cinnamamide	-46.4 ± 0.1	-32.5 ± 0.1	-55.0 ± 0.4
3510	(4-bromobenzyl)propanedinitrile	-28.2 ± 0.1	-49.5 ± 0.2	-55.5 ± 0.3
3517	2-chloro-1-4-napthoquinone	-30.7 ± 0.1	-40.3 ± 0.1	-48.4 ± 0.3
3555	(2-4-dichlorobenzyl)malonamide	-71.6 ± 0.4	-50.8 ± 0.2	-82 ± 1
3799	nicotine	-29.2 ± 0.1	-37.8 ± 0.1	-47.5 ± 0.3
4027	2-methylbenzal malonamide	-50.8 ± 0.1	-44.4 ± 0.1	-68 ± 1
4059	ethyl cinnamate	-24.5 ± 0.1	-37.5 ± 0.1	-45.8 ± 0.3
4299	(4-bromo-benzal)-acetylacetone	-47.9 ± 0.1	-47.4 ± 0.2	-64.5 ± 0.5
4312	ethyl benzalcyanoacetate	-33.8 ± 0.1	-45.7 ± 0.2	-54.9 ± 0.3
4712	2-butylthio-1-4-naphthoquinone	-28.6 ± 0.1	-53.3 ± 0.2	-59.7 ± 0.3
4764	1-cinnamoylpiperidine	-40.4 ± 0.1	-50.4 ± 0.2	-67.2 ± 0.4
5785	erythromycin	-117.2 ± 0.3	-122.6 ± 0.4	-153 ± 1

Table 1: Complete list of calculated solvation free energies in kJ/mol for all solutes in water, cyclohexane, and octanol using GAFF

DB num.	Name	Solvation Free Energy (kJ/mol)		
		Water	Cyclohexane	Octanol
159	methanol	-22.7 ± 0.1	-3.7 ± 0.1	-19.8 ± 0.3
492	acetone	-14.9 ± 0.1	-10.0 ± 0.1	-16.8 ± 0.3
671	trimethylamine	-11.2 ± 0.1	-12.1 ± 0.1	-18.2 ± 0.2
835	2-2-2-trichloro-1-dimethoxyphosphorylethanol	-61.3 ± 0.1	-42.5 ± 0.1	-72 ± 1
950	butanol	-21.3 ± 0.1	-14.7 ± 0.1	-30.1 ± 0.3
1014	butylamine	-12.6 ± 0.1	-15.1 ± 0.1	-16.0 ± 0.2
1028	diethylamine	-12.5 ± 0.1	-15.2 ± 0.1	-22.3 ± 0.2
1307	pentachlorophenol	-20.8 ± 0.1	-44.0 ± 0.1	-61.4 ± 0.4
1363	quinone	-29.1 ± 0.1	-23.7 ± 0.1	-30.8 ± 0.2
1425	p-iodophenol	-32.0 ± 0.1	-30.2 ± 0.1	-50.8 ± 0.4
1453	o-nitrophenol	-28.5 ± 0.1	-33.3 ± 0.1	-43.9 ± 0.4
1711	aniline	-23.0 ± 0.1	-19.8 ± 0.1	-24.2 ± 0.2
1879	nitrocyclohexane	-9.8 ± 0.1	-31.8 ± 0.1	-31.4 ± 0.3
2133	benzaldehyde	-21.2 ± 0.1	-21.7 ± 0.1	-26.7 ± 0.2
2185	salicylic acid	-37.1 ± 0.2	-31.7 ± 0.1	-47.6 ± 0.3
2323	m-methylphenol	-29.5 ± 0.1	-22.3 ± 0.1	-43.2 ± 0.3
2336	o-methylphenol	-28.0 ± 0.1	-22.2 ± 0.1	-41.1 ± 0.4
2348	p-methylphenol	-30.3 ± 0.1	-22.4 ± 0.1	-41.6 ± 0.3
2411	o-toluidine	-22.6 ± 0.1	-22.8 ± 0.1	-25.2 ± 0.2
2422	p-toluidine	-22.7 ± 0.1	-22.9 ± 0.1	-30.5 ± 0.3
2612	phthalimide	-50.0 ± 0.1	-36.3 ± 0.1	-51.9 ± 0.3
2790	vanillin	-38.4 ± 0.1	-33.5 ± 0.1	-45.0 ± 0.3
2914	2-4-dimethylphenol	-27.5 ± 0.1	-25.6 ± 0.1	-41.3 ± 0.4
2917	2-5-dimethylphenol	-27.5 ± 0.1	-25.5 ± 0.1	-37.5 ± 0.3
2925	3-4-dimethylphenol	-29.5 ± 0.1	-25.5 ± 0.1	-45.2 ± 0.3
2938	p-ethylphenol	-29.5 ± 0.1	-25.4 ± 0.1	-45.0 ± 0.3
3110	5-cyano-2-(trifluoromethyl)-1h-benzimidazole	-45.5 ± 0.1	-44.0 ± 0.1	-70.7 ± 0.3
3126	coumarin	-34.2 ± 0.1	-33.3 ± 0.1	-48.8 ± 0.4
3130	1-3-indanedione	-31.8 ± 0.1	-33.3 ± 0.1	-39.8 ± 0.3
3228	cinnamamide	-46.4 ± 0.1	-32.5 ± 0.1	-57.6 ± 0.3
3510	(4-bromobenzyl)propanedinitrile	-28.2 ± 0.1	-49.5 ± 0.2	-53.7 ± 0.4
3517	2-chloro-1-4-napthoquinone	-30.7 ± 0.1	-40.3 ± 0.1	-47.0 ± 0.3
3555	(2-4-dichlorobenzyl)malonamide	-71.6 ± 0.4	-50.8 ± 0.2	-71.6 ± 0.4
3799	nicotine	-29.2 ± 0.1	-37.8 ± 0.1	-44.3 ± 0.4
4027	2-methylbenzal malonamide	-50.8 ± 0.1	-44.4 ± 0.1	-65 ± 1
4059	ethyl cinnamate	-24.5 ± 0.1	-37.5 ± 0.1	-41.9 ± 0.3
4299	(4-bromo-benzal)-acetylacetone	-47.9 ± 0.1	-47.4 ± 0.2	-65 ± 1
4312	ethyl benzalcyanoacetate	-33.8 ± 0.1	-45.7 ± 0.2	-46.9 ± 0.4
4712	2-butylthio-1-4-naphthoquinone	-28.6 ± 0.1	-53.3 ± 0.2	-57.2 ± 0.4
4764	1-cinnamoylpiperidine	-40.4 ± 0.1	-50.4 ± 0.2	-68.4 ± 0.4
5785	erythromycin	-129.0 ± 0.3	-123.0 ± 0.4	-155 ± 1

Table 2: Complete list of calculated solvation free energies in kJ/mol for all solutes in water, cyclohexane, and octanol using GAFF-DC

DB num.	Name	Cyclohexane Partition Coefficients		
		GAFF	GAFF-DC	Literature
159	methanol	-1.90 ± 0.01	-3.32 ± 0.01	-1.84
492	acetone	-0.85 ± 0.02	-0.85 ± 0.02	-0.96
671	trimethylamine	0.16 ± 0.02	0.16 ± 0.02	-0.44
835	2-2-2-trichloro-1-dimethoxyphosphorylethanol	-2.31 ± 0.03	-3.29 ± 0.03	-1.70
950	butanol	0.17 ± 0.02	-1.16 ± 0.02	-0.72
1014	butylamine	0.44 ± 0.02	0.44 ± 0.02	-0.29
1028	diethylamine	0.46 ± 0.02	0.46 ± 0.02	-0.34
1307	**pentachlorophenol**	5.06 ± 0.03	4.07 ± 0.03	-0.52
1363	quinone	-0.94 ± 0.02	-0.94 ± 0.02	-0.39
1425	p-iodophenol	0.89 ± 0.02	-0.31 ± 0.03	0.00
1453	o-nitrophenol	1.90 ± 0.03	0.84 ± 0.03	1.49
1711	aniline	-0.56 ± 0.02	-0.56 ± 0.02	0.98
1879	**nitrocyclohexane**	3.86 ± 0.03	3.86 ± 0.03	-0.10
2133	benzaldehyde	0.10 ± 0.02	0.10 ± 0.02	1.13
2185	salicylic acid	0.66 ± 0.03	-0.95 ± 0.04	-1.02
2323	m-methylphenol	-0.10 ± 0.02	-1.27 ± 0.02	-0.30
2336	o-methylphenol	0.18 ± 0.02	-1.01 ± 0.02	0.04
2348	p-methylphenol	-0.14 ± 0.02	-1.39 ± 0.02	-0.10
2411	o-toluidine	0.03 ± 0.02	0.03 ± 0.02	0.67
2422	p-toluidine	0.03 ± 0.02	0.03 ± 0.02	0.58
2612	phthalimide	-2.41 ± 0.02	-2.41 ± 0.02	-1.46
2790	vanillin	-0.09 ± 0.03	-0.86 ± 0.03	-0.75
2914	2-4-dimethylphenol	0.89 ± 0.03	-0.35 ± 0.03	0.76
2917	2-5-dimethylphenol	0.76 ± 0.03	-0.34 ± 0.03	0.77
2925	3-4-dimethylphenol	0.49 ± 0.03	-0.70 ± 0.03	0.20
2938	p-ethylphenol	0.49 ± 0.03	-0.72 ± 0.03	0.44
3110	5-cyano-2-(trifluoromethyl)-1h-benzimidazole	-0.27 ± 0.03	-0.27 ± 0.03	-1.15
3126	coumarin	-0.17 ± 0.03	-0.17 ± 0.03	0.48
3130	1-3-indanedione	0.27 ± 0.03	0.27 ± 0.03	-0.12
3228	cinnamamide	-2.43 ± 0.03	-2.43 ± 0.03	-2.21
3510	(4-bromobenzyl)propanedinitrile	3.72 ± 0.03	3.72 ± 0.03	2.03
3517	2-chloro-1-4-napthoquinone	1.67 ± 0.03	1.67 ± 0.03	1.91
3555	(2-4-dichlorobenzyl)malonamide	-3.63 ± 0.08	-3.6 ± 0.1	-3.32
3799	nicotine	1.50 ± 0.03	1.50 ± 0.03	0.25
4027	2-methylbenzal malonamide	-1.12 ± 0.03	-1.12 ± 0.03	-2.86
4059	ethyl cinnamate	2.28 ± 0.03	2.28 ± 0.03	3.27
4299	(4-bromo-benzal)-acetylacetone	-0.08 ± 0.04	-0.08 ± 0.04	1.82
4312	ethyl benzalcyanoacetate	2.08 ± 0.03	2.08 ± 0.03	2.63
4712	2-butylthio-1-4-naphthoquinone	4.32 ± 0.04	4.32 ± 0.04	3.43
4764	1-cinnamoylpiperidine	1.76 ± 0.04	1.76 ± 0.04	1.44
5785	erythromycin	0.95 ± 0.09	-1.0 ± 0.1	-0.22

All experimental $\log P_{cyc}$ are from Albert Leo et al. *Chem. Rev.* **1971,** 71, 525-616.

Table 3: Complete list of calculated and experimental $\log P_{cyc}$ in GAFF and GAFF-DC where applicable. There are blanks for non-alcohols in GAFF-DC as the change in parameters only affects molecules with hydroxyl groups. Outliers by more than 3 log units are indicated in bold

DB num.	Name	Octanol Partition Coefficient			
		GAFF	GAFF-DC	OExLogP	Literature
159	methanol	-0.29 ± 0.03	-0.50 ± 0.05	-0.56	-0.66
492	acetone	0.20 ± 0.03	0.33 ± 0.05	0.26	-0.24
671	trimethylamine	1.09 ± 0.03	1.23 ± 0.03	0.44	0.27
835	2-2-2-trichloro-1-dimethoxyphosphorylethanol	2.26 ± 0.09	1.8 ± 0.1	1.95	0.51
950	butanol	1.58 ± 0.03	1.5 ± 0.1	0.83	0.88
1014	butylamine	1.22 ± 0.03	0.60 ± 0.04	0.94	0.88
1028	diethylamine	1.43 ± 0.03	1.72 ± 0.04	0.85	0.57
1307	pentachlorophenol	6.53 ± 0.05	7.1 ± 0.1	4.16	5.01
1363	quinone	0.62 ± 0.05	0.31 ± 0.04	0.48	0.20
1425	p-iodophenol	3.53 ± 0.04	3.3 ± 0.1	2.18	2.91
1453	o-nitrophenol	2.58 ± 0.06	2.7 ± 0.1	-0.28	1.79
1711	aniline	0.63 ± 0.04	0.22 ± 0.04	1.19	0.90
1879	nitrocyclohexane	3.95 ± 0.04	3.8 ± 0.1	0.67	
2133	benzaldehyde	1.47 ± 0.04	0.98 ± 0.05	1.63	1.48
2185	salicylic acid	2.33 ± 0.05	1.8 ± 0.1	0.76	2.26
2323	m-methylphenol	1.80 ± 0.04	2.4 ± 0.1	1.37	1.96
2336	o-methylphenol	1.89 ± 0.05	2.3 ± 0.1	1.37	1.95
2348	p-methylphenol	1.98 ± 0.04	1.97 ± 0.05	1.37	1.94
2411	o-toluidine	1.10 ± 0.04	0.45 ± 0.04	1.48	1.29
2422	p-toluidine	1.26 ± 0.04	1.4 ± 0.1	1.49	1.39
2612	phthalimide	1.36 ± 0.07	0.3 ± 0.1	0.69	1.15
2790	vanillin	1.70 ± 0.05	1.1 ± 0.1	0.82	1.21[a]
2914	2-4-dimethylphenol	2.37 ± 0.04	2.4 ± 0.1	1.67	2.35[b]
2917	2-5-dimethylphenol	2.29 ± 0.06	1.8 ± 0.1	1.67	2.34[b]
2925	3-4-dimethylphenol	2.41 ± 0.05	2.7 ± 0.1	1.67	2.23[b]
2938	p-ethylphenol	2.37 ± 0.04	2.7 ± 0.1	1.73	2.50[b]
3110	5-cyano-2-(trifluoromethyl)-1h-benzimidazole	4.25 ± 0.06	4.4 ± 0.1	2.25	
3126	coumarin	2.39 ± 0.06	2.6 ± 0.1	1.72	1.39
3130	1-3-indanedione	1.82 ± 0.05	1.4 ± 0.1	0.94	0.36
3228	cinnamamide	1.52 ± 0.07	1.97 ± 0.05	1.46	1.43[b]
3510	(4-bromobenzyl)propanedinitrile	4.79 ± 0.05	4.5 ± 0.1	2.32	
3517	2-chloro-1-4-napthoquinone	3.10 ± 0.05	2.9 ± 0.1	2.26	2.15
3555	(2-4-dichlorobenzyl)malonamide	1.83 ± 0.20	0.0 ± 0.1	1.40	
3799	nicotine	3.19 ± 0.06	2.6 ± 0.1	1.50	1.17
4027	2-methylbenzal malonamide	3.00 ± 0.21	2.5 ± 0.2	0.94	
4059	ethyl cinnamate	3.73 ± 0.05	3.0 ± 0.1	2.85	2.99[a]
4299	(4-bromo-benzal)-acetylacetone	2.92 ± 0.09	3.0 ± 0.1	2.98	2.75[a]
4312	ethyl benzalcyanoacetate	3.69 ± 0.06	2.3 ± 0.1	2.38	2.43[a]
4712	2-butylthio-1-4-naphthoquinone	5.44 ± 0.06	5.0 ± 0.1	3.62	3.29
4764	1-cinnamoylpiperidine	4.70 ± 0.07	4.9 ± 0.1	3.12	2.74[a]
5785	**erythromycin**	6.30 ± 0.16	4.6 ± 0.2	**2.65**	2.48

[a] experimental $\log P_{oct}$ from Corwin Hansch et al. *Exploring QSAR: Hydrophobic, Electronic, and Steric Constants* **1995.**
[b] experimental $\log P_{oct}$ from James Sangster *J. Phys. Chem. Ref. Data* **1989,** 18, 111-1227.
All other experimental $\log P_{oct}$ are from Albert Leo et al. *Chem. Rev.* **1971**, 71, 525-616.

Table 4: Complete list of calculated and experimental $\log P_{oct}$ in GAFF and GAFF-DC. A blank indicates the data is unavailable, for 5 solutes experimental data for $\log P_{oct}$ has not been located. Outliers by more than 3 log units are indicated in bold

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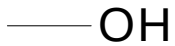	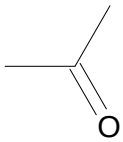	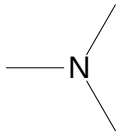	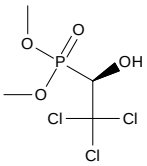	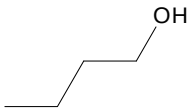	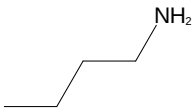
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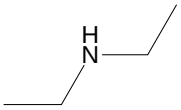	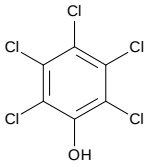	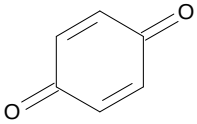	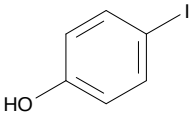	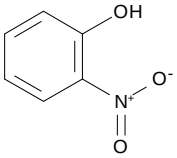	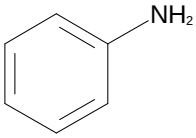
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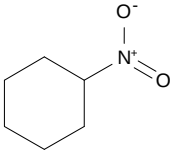	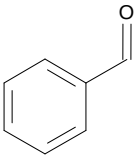	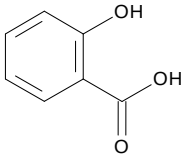	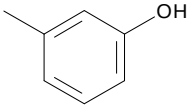	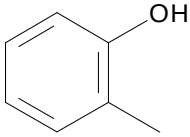	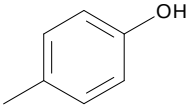
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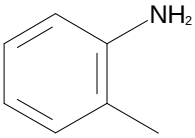	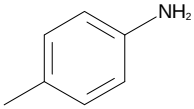	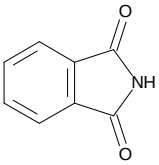	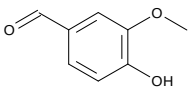	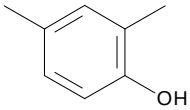	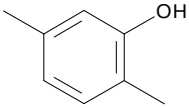
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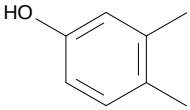	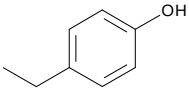	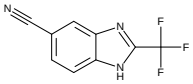	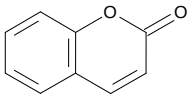	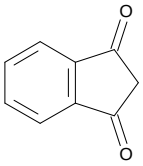	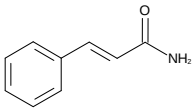
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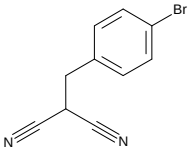	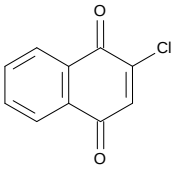	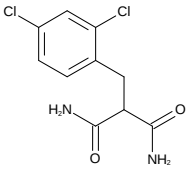	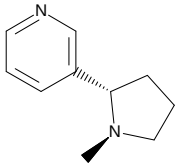	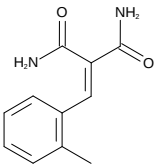	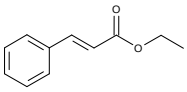
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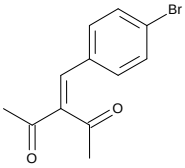	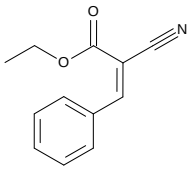	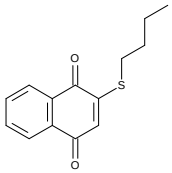	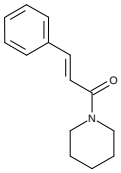	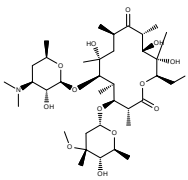	

Table 5: This table is a complete list of molecules used in this study with their database number.