

**Competitor Analysis of Functional Group H-bond Donor and Acceptor
Properties Using the Cambridge Structural Database**

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Supplementary Information

Table S1. Experimentally determined solution phase H-bond donor parameters, average functional group values and standard deviations.

Functional Group	SMARTS string	Compounds	α
Primary alcohol	[CX4](C(O[H])([H])[H])([!F!Cl!Br!I])([!F!Cl!Br!I])[!F!Cl!Br!I]	Ethanol	2.72
		Butan-1-ol	2.71
		Hexan-1-ol	2.70
		Neopentanol	2.68
		Propan-1-ol	2.65
		Average	2.69
		Standard deviation	0.03
Benzyl primary alcohol	c(C(O[H])([H])[H])	Benzyl alcohol	2.96
		Average	2.96
		Standard deviation	0.00
Halogenated primary alcohol	[CX4](C)([H])([FClBrI])(C(O[H])([H])[H])	2-Chloroethanol	3.28
		2-Fluoroethanol	2.97
		Average	3.13
		Standard deviation	0.22
Methanol	C(O[H])([H])([H])[H]	Methanol	2.86
		Average	2.86
		Standard deviation	0.00
Water	O([H])[H]	Water	2.80
		Average	2.80
		Standard deviation	0.00
Secondary alcohol	C(O[H])([Cc])([Cc])[H]	Propan-2-ol	2.69
		Cyclohexanol	2.58

		Cholesterol	2.62
		Butan-2-ol	2.54
		Average	2.61
		Standard deviation	0.06
Tertiary alcohol	<chem>C([CX4])([CX4])([CX4])O[H]</chem>	tert-Butyl alcohol	2.67
		tert-Pentanol	2.65
		Average	2.66
		Standard deviation	0.01
Primary aniline	<chem>c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!!O!N]))[!F!Cl!Br!!O!N])N([H])[H])[!F!Cl!Br!!O!N])[!F!Cl!Br!!O!N])[!F!Cl!Br!!O!N]</chem>	β -Naphthylamine	2.78
		Aniline	2.40
		α -Naphthylamine	2.60
		Average	2.62
		Standard deviation	0.17
Secondary aniline	<chem>c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!!O!N]))[!F!Cl!Br!!O!N])N([CX4])[H])[!F!Cl!Br!!O!N])[!F!Cl!Br!!O!N])[!F!Cl!Br!!O!N]</chem>	N-Methylaniline	2.06
		Average	2.06
		Standard deviation	0.00
Diphenyl aniline	<chem>c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!!O!N]))[!F!Cl!Br!!O!N])N(c:2:c(:c(:c(:c:2[!F!Cl!Br!!O!N]))[!F!Cl!Br!!O!N])[!F!Cl!Br!!O!N])[!F!Cl!Br!!O!N])[H])[!F!Cl!Br!!O!N])[!F!Cl!Br!!O!N]</chem>	Diphenylaniline	2.68
		Average	2.68
		Standard deviation	0.00
Oxime	<chem>N(=C([cCX4])[cCX4])O[H]</chem>	4a-phenyloctahydronaphthalen-2(1)-one oxime	3.00

		Average	3.00
		Standard deviation	0.00
Alkyl carboxylic acid	C(=O)(O[H])[CX4]	Acetic acid	3.61
		tert-Butanoic acid	3.46
		Hexanoic acid	3.28
		Average	3.45
		Standard deviation	0.16
Aryl carboxylic acid	C(=O)(O[H])[c]	Benzoic acid	3.76
		Average	3.76
		Standard deviation	0.00
Secondary amide N alkyl	[CX4](=O)(C)N([H])[CX4]	N-Methylacetamide	2.92
		N-hexylheptamide	2.79
		Average	2.86
		Standard deviation	0.10
Secondary amide N aryl	C(=O)([CX4])N([H])c	Acetanilide	3.30
		Average	3.30
		Standard deviation	0.00
Formamide	C(=O)([H])N([H])[CX4]	N-Methylformamide	2.90
		Average	2.90
		Standard deviation	0.00
Imide	N(C(=O)[CX4cCX3])([H])C(=O)[CX4cCX3]	Maleimide	3.39
		Succinimide	3.37
		Average	3.38

		Standard deviation	0.01
phenol	c:1(:c(:c(:c(:c(:c:1[CcH])[CcH])O[H]))[CcH])[CcH])[CcH]	2-Naphthol	3.90
		1-Naphthol	3.80
		Phenol	3.80
		4-Phenylphenol	3.80
		3-Isopropylphenol	3.70
		4-sec-Butylphenol	3.70
		3-Methylphenol	3.70
		4-Methylphenol	3.70
		3_5-Dimethylphenol	3.70
		4-Methyl-2-tert-butylphenol	3.70
		3_4-Dimethylphenol	3.60
		4-tert-Butylphenol	3.60
		3-Methyl-6-tert-butylphenol	3.60
		3-Ethylphenol	3.60
		4-Octylphenol	3.60
		4-Ethylphenol	3.60
		4-Propylphenol	3.60
		3_4_5-Trimethylphenol	3.60
		2_4-di-tert-butylphenol	3.60
		2_5-Dimethylphenol	3.60
		2_3-Dimethylphenol	3.50
		2_4-Dimethylphenol	3.50
		2_3_5-Trimethylphenol	3.50
		2-Methylphenol	3.50
		2-tert-Butylphenol	3.40
		Average	3.64
		Standard Deviation	0.12
Ortho halogenated phenol	c:1(:c(:c(:c(:c(:c:1[CcH1])[CcH1])O[H]))[FCIBrI])[CcH1])[CcH1]	2-Chlorophenol	4.02
		Average	4.02
		Standard Deviation	0.00
Meta halogenated phenol	c:1(:c(:c(:c(:c(:c:1[CcH1])[CcH1])O[H]))[CcH1])[FCIBrI])[CcH1]	3-Bromophenol	4.22

		3-Chlorophenol	4.19
		3-Fluorophenol	4.13
		Average	4.18
		Standard Deviation	0.05
Para halogenated phenol	<chem>c:1(:c(:c(:c(:c:1[CcH1])[CcH1])O[H])[CcH1])[CcH1])[FCIBrI]</chem>	4-Iodophenol	4.14
		4-Bromophenol	4.11
		4-Chlorophenol	4.10
		4-Fluorophenol	3.93
		Average	4.07
		Standard Deviation	0.09
Thiol	<chem>[CX4]S[H]</chem>	Propyl sulphide	1.44
		Ethyl sulphide	1.39
		Butyl sulphide	1.28
		Isopropyl sulphide	1.28
		t-Butyl sulphide	1.28
		Average	1.33
		Standard Deviation	0.07
Secondary Thioamide	<chem>C(=S)([cCX4])N([CX4c])[H]</chem>	Thioacetamide	3.70
		Thioacetanilide	3.40
		Average	3.55
		Standard Deviation	0.21
Secondary Sulphonamide	<chem>[cC]S(=O)(=O)N([H])([cC])</chem>	N-(2-Naphthyl)toluene-p-sulfonamide	3.20
		Toluene-p-sulfonamide	3.20
		N-Benzyltoluene-p-sulfonamide	3.00
		Average	3.13
		Standard Deviation	0.12
Thiophenol	<chem>c:1:c:c(:c:c:1)S[H]</chem>	Thiophenol	1.40

		Average	1.40
		Standard Deviation	0.00
Secondary carbamate N aryl	<chem>O(C(=O)N([H])[c])[CX4]</chem>	N-Phenylurethane	2.82
		Average	2.82
		Standard Deviation	0.00
Thiourea N alkyl NN alkyl	<chem>C(=S)(N([CX4])[H])N([CX4])[CX4]</chem>	N-Methyl-N_N'-propylenethiourea	3.03
		Average	3.03
		Standard Deviation	0.00
Pyrrole	<chem>N1(C(=C(C(=C1[CX4H])[CX4H])[CX4H])[CX4H])[H]</chem>	Pyrrole	3.02
		Average	3.03
		Standard Deviation	0.00
Indole	<chem>N1(C=Cc:2c1:c:c:c:2)[H]</chem>	Indole	3.14
		Average	3.14
		Standard Deviation	0.00
Pyrazole	<chem>N1=CC=CN1[H]</chem>	pyrazole	3.61
		3-methylpyrazole	3.57
		5-methylpyrazole	3.57
		3_5-dimethylpyrazole	3.57
		4-methylpyrazole	3.53
		3_4_5-trimethylpyrazole	3.36
		Average	3.53
		Standard Deviation	0.09
1,2,3 Triazole	<chem>N1=CC=NN1[H]</chem>	3-Methylthio-1_2_3-Triazole	3.94
		4-Trifluoromethane-1_2_3-triazole	4.34

		Average	4.14
		Standard Deviation	0.28
1,3,4 Triazole	C1=NC=NN1[H]	3-Triazolepropylphenyl	3.80
		Average	3.80
		Standard Deviation	0.00
Tetrazole	N1=NN=CN1[H]	5-Phenyl-1_2_3_4-tetrazole	4.97
		Average	3.53
		Standard Deviation	0.09

Table S2. Experimentally determined solution phase H-bond acceptor parameters, average functional group values and standard deviations.

Functional Group	SMARTS string	Compounds	β
Primary alcohol	[CX4](C(O[H])([H])[H])([!F!Cl!Br!I])([!F!Cl!Br!I])[!F!Cl!Br!I]	Octan-1-ol	5.36
		Propan-1-ol	5.25
		Ethanol	5.15
		Average	5.25
		Standard Deviation	0.10
Benzyl primary alcohol	c(C(O[H])([H])[H])	Benzyl alcohol	4.94
		Average	4.94
		Standard Deviation	0.00
Halogenated primary alcohol	[CX4](C)([H])([FClBrI])(C(O[H])([H])[H])	2-Fluoroethanol	4.33
		2-Bromoethanol	4.22
		2-Chloroethanol	4.22
		Average	4.26
		Standard Deviation	0.06
Methanol	C(O[H])([H])([H])[H]	Methanol	4.84
		Average	4.84
		Standard Deviation	0.00
Water	O([H])[H]	Water	4.50
		Average	4.50
		Standard Deviation	0.00
Secondary alcohol	C(O[H])([Cc])([Cc])[H]	Cyclohexanol	5.56
		Propan-2-ol	5.46

		Average	5.51
		Standard Deviation	0.07
Tertiary alcohol	<chem>C([cC])([cC])([cC])O[H]</chem>	Tert-butyl alcohol	5.70
		Average	5.70
		Standard Deviation	0.00
Alkyl alkyl ether	<chem>C(OC([!c])([!c])[!c])([!c])([!c])[!c]</chem>	2-Methyltetrahydrofuran	6.00
		Tetrahydrofuran	5.90
		Tetrahydropyran	5.80
		tert-Butyl methyl ether	5.70
		Diisopropyl ether	5.50
		tert-Butyl ethyl ether	5.50
		Dipentyl ether	5.40
		Diethyl ether	5.30
		Dipropyl ether	5.20
		n-Propylethylether	5.20
		Dimethyl ether	5.10
		Dibutyl ether	5.00
		Average	5.55
		Standard Deviation	0.33
Allyl ether	<chem>C(OC([!c])([!c])(C=C))([!c])(C=C)[!c]</chem>	Diallyl ether	4.60
		Average	4.60
		Standard Deviation	0.00
Alkyl aryl ether	<chem>cO[CX4]</chem>	Anisole	3.30
		Average	3.30
		Standard Deviation	0.00
Alkyl alkyl ether benzyl	<chem>O(C(C:1:c:c:c:c:1)([H])[H])C(C:2:c:c:c:c:2)([H])[H]</chem>	Dibenzyl ether	4.50

		Average	3.30
		Standard Deviation	0.00
Aryl aryl ether	cOc	Diphenyl ether	3.10
		Average	3.10
		Standard Deviation	0.00
Lactone	[CX4]1C[CX4]C(O1)=O	δ -Valerolactone	6.55
		γ -Valerolactone	6.24
		γ -Butyrolactone	5.99
		Average	6.26
		Standard Deviation	0.28
Vinyl ester	C=C([H])OC(=O)([CX4])	Vinyl Acetate	4.72
		Average	4.72
		Standard Deviation	0.00
Carbonate	[CX4c]OC(=O)O[CX4c]	S-ethyl methyl carbonate	4.68
		Average	4.68
		Standard Deviation	0.00
Formate	[H]C(=O)O([CX4])	Ethyl formate	4.53
		Methyl formate	4.52
		Phenylformate	4.51
		Average	4.52
		Standard Deviation	0.01
Oxalate	[Cc]OC(=O)(C(=O)(O[cC]))	Diethyl oxalate	4.51
		Average	4.51
		Standard Deviation	0.00
Coumarin	O1C(=O)C=CC=C1	Coumarin	5.95

		Average	5.95
		Standard Deviation	0.00
Anhydride	[CX4c]C(=O)OC(=O)[CX4c]	Acetic anhydride	6.40
		Average	6.40
		Standard Deviation	0.00
Tri halo esters	C(C(=O)O[Cc])([FClBrI])([FClBrI])[FClBrI]	Ethyl trichloroacetate	3.40
		Methyl trichloroacetate	3.31
		Ethyl trifluoroacetate	3.24
		Average	3.31
		Standard Deviation	0.08
Benzoate	c:1:c:c(:c:c:c:1)C(=O)O[CX4]	Ethyl 3-methylbenzoate	5.31
		tert-Butyl benzoate	5.22
		Ethyl benzoate	5.15
		Ethyl 4-cyanobenzoate	5.06
		Methyl benzoate	5.04
		Ethyl 4-fluorobenzoate	5.02
		Average	5.13
		Standard Deviation	0.11
Mono halogenated ester	[CX4]C(=O)O[CX4]([CH])([CH])[FClBrI]	Ethyl fluoroacetate	4.71
		Ethyl chloroacetate	4.55
		Average	4.63
		Standard Deviation	0.11
Alkyl alkyl ester	[CX4!R]C(=O)O[CX4!R]	sec-Butyl acetate	5.64
		Propyl ethanoate	5.62
		Isopropyl ethanoate	5.62
		Isobutyl acetate	5.59
		(E)-Ethyl cinnamate	5.59
		Butyl acetate	5.57
		Ethyl 4-methoxybenzoate	5.57

		Methyl-cyclopropanecarboxylate	5.55
		Ethyl cyclopropanecarboxylate	5.55
		Ethyl isovalerate	5.53
		Ethyl butyrate	5.53
		tert-Butyl ethanoate	5.51
		Ethyl isobutyrate	5.48
		Ethyl propionate	5.46
		Ethyl ethanoate	5.44
		Methyl cyclohexanecarboxylate	5.42
		Ethyl 1-adamantanecarboxylate	5.42
		Ethyl 4-methylbenzoate	5.39
		Ethyl phenylacetate	5.39
		Ethyl 2_2-dimethylpropanoate	5.37
		Average	5.51
		Standard Deviation	0.08
Primary amine	N([H])([H])C([H])([H])[CX4]	Adamantan-1-amine	8.19
		c-Hexylamine	8.15
		Octadecylamine	8.14
		n-octylamine	8.11
		tert-butylamine	8.08
		n-Hexadecylamine	8.08
		Isopropylamine	7.99
		n-Butylamine	7.97
		ethylamine	7.88
		Methylamine	7.84
		Hexylamine	7.73
		Heptylamine	7.73
		Average	7.99
		Standard Deviation	0.16
Primary benzyl amine	N([H])([H])C([H])([H])c	3-methylbenzylamine	7.44
		benzylamine	7.24
		Average	7.34
		Standard Deviation	0.14

Allyl amine		Allylamine	7.37
		Average	7.37
		Standard Deviation	0.10
Acyclic secondary amine	<chem>N([H])([CX4!R1])([!c])([!c])[!c][CX4!R1]([!c])([!c])[!c]</chem>	dimethylamine	8.10
		N-methylethylamine	8.10
		Dipropylamine	7.90
		Dibutylamine	7.90
		Dipentylamine	7.90
		Average	7.98
		Standard Deviation	0.11
Cyclic secondary amine	<chem>[NR]([H])([CX4R])([CX4R])</chem>	pyrrolidine	8.80
		azetidine	8.80
		piperidine	8.30
		Average	8.63
		Standard Deviation	0.29
Dibenzyl secondary amine	<chem>N([H])([CX4!R1])([!c])([!c])[c][CX4!R1]([!c])([!c])[c]</chem>	Dibenzylamine	6.27
		Average	6.27
		Standard Deviation	0.00
Tertiary amine	<chem>N([CX4]([!c])([!c])[!c])([CX4]([!c])([!c])[!c])([CX4]([!c])([!c])[!c])</chem>	trimethylamine	7.79
		N-methylpiperidine	7.75
		Triethylamine	7.51
		Trioctylamine	7.00
		Tributylamine	6.77
		Tripentylamine	6.90
		Average	7.29
		Standard Deviation	0.45

Triallyl amine	<chem>N([C]([C])C=C)([C]([C])C=C)([C]([C])C=C)</chem>	Triallylamine	6.14
		Average	6.14
		Standard Deviation	0.00
Tribenzyl amine	<chem>N([C]([C])c)([C]([C])c)([C]([C])c)</chem>	Tribenzylamine	3.79
		Average	3.79
		Standard Deviation	0.00
Primary aniline	<chem>c1(:c(:c(:c(:c1[F]ClBrIO[N])[F]ClBrIO[N])N([H])[H])[F]ClBrIO[N])[F]ClBrIO[N])[F]ClBrIO[N]</chem>	4-Methylaniline	4.94
		3-Methylaniline	4.69
		2-Methylaniline	4.53
		Aniline	4.51
		Average	4.67
		Standard Deviation	0.20
Para halogenated primary aniline	<chem>c1(:c(:c(:c(:c1[F]ClBrIO[N])[F]ClBrIO[N])N([H])[H])[F]ClBrIO[N])[F]ClBrIO[N])[FCIBr]</chem>	4-Fluoroaniline	4.35
		4-Chloroaniline	4.10
		4-Bromoaniline	4.08
		4-Iodoaniline	3.84
		Average	4.09
		Standard Deviation	0.21
Ortho halogenated primary aniline	<chem>c1(:c(:c(:c(:c1[F]ClBrIO[N])[F]ClBrIO[N])N([H])[H])[F]ClBrIO[N])[FCIBrI])[F]ClBrIO[N]</chem>	3-Fluoroaniline	3.74
		3-Chloroaniline	3.58
		3-Iodoaniline	3.58
		3-Bromoaniline	3.44
		Average	3.59

		Standard Deviation	0.12
Alkyl alkyl tertiary aniline	c:1:c:c:c(:c:c:1)N([CX4])[CX4]	N_N-Diethylaniline	4.90
		N_N-Dimethylaniline	4.20
		Average	4.55
		Standard Deviation	0.49
Alkyl aldehyde	C(=O)([H])[CX4]	Butanaldehyde	4.70
		Decanaldehyde	4.70
		Propanaldehyde	4.60
		Octanaldehyde	4.60
		Acetaldehyde	4.50
		Average	4.62
		Standard Deviation	0.08
Aryl aldehyde	C(=O)([H])[c]	Benzaldehyde	4.80
		Average	4.80
		Standard Deviation	0.00
Cyclic ketone	[CX4R][CR](=O)[CX4R]	Cyclooctanone	6.28
		Cycloheptanone	6.19
		Cyclohexanone	6.15
		Camphor	5.97
		1-Adamantyl methyl ketone	5.95
		Cyclopentanone	5.88
		2-Methylcyclohexanone	5.88
		Cyclododecanone	5.79
		Cyclopentadecanone	5.77
		Cycloundecanone	5.73
		Average	5.96
		Standard Deviation	0.19
Acetophenone	C(=O)([CX4])c:1:c:c:c:c:1	4-(1-Adamantyl)acetophenone	5.95
		4-tert-Butylacetophenone	5.84

		4-Ethylacetophenone	5.84
		4-Methylacetophenone	5.82
		4-Isopropylacetophenone	5.75
		Acetophenone	5.53
		3-Methylacetophenone	5.51
		Average	5.75
		Standard Deviation	0.17
Acyclic dialkyl ketone	<chem>C(=O)([CX4!R]([!c])([!c])[!c])[CX4!R]([!c])([!c])[!c]</chem>	Cyclohexyl methyl ketone	5.82
		3-Methylpentan-2-one	5.77
		Butan-2-one	5.77
		3-Methylbutan-2-one	5.73
		Hexan-2-one	5.68
		Propan-2-one	5.68
		4-Methylpentan-2-one	5.66
		Pentan-2-one	5.66
		Di-(1-adamantyl)ketone	5.66
		Pentan-3-one	5.59
		Heptan-4-one	5.59
		Hexan-3-one	5.57
		Methyl isopropyl ketone	5.63
		Average	5.68
		Standard Deviation	0.07
Diaryl ketone	<chem>C(=O)(c:1:c:c:c:c:1)c:2:c:c:c:c:2</chem>	Benzophenone	5.44
		Anthrone	5.64
		Average	5.54
		Standard Deviation	0.14
Dibenzyl ketone	<chem>[C!R](=O)([CX4]c)([CX4]c)</chem>	Dibenzyl ketone	5.30
		Average	5.54
		Standard Deviation	0.14
Mono halogenated ketone	<chem>[C!R](=O)([CX4!R])C(Cl)([CH])[C H]</chem>	Chloropropan-2-one	4.53

		Average	4.53
		Standard Deviation	0.00
Tri halogenated ketone	<chem>C(=O)([CX4!R])C([FClBrI])([FClBrI])([FClBrI])</chem>	1_1_1-Trichloropropan-2-one	3.06
		1_1_1-Trifluoropropan-2-one	2.93
		Average	3.00
		Standard Deviation	0.09
Cyclohexene-one	<chem>C1C=CC([CX4]C1)=O</chem>	Piperitone	6.14
		Average	6.14
		Standard Deviation	0.00
O aryl substituted Oxime	<chem>cON=C([cCX4])([cCX4])</chem>	Acetone O-phenyloxime	4.77
		Average	4.77
		Standard Deviation	0.00
O alkyl substituted Oxime	<chem>[CX4]ON=C([cCX4])([cCX4])</chem>	(1E)-Cyclohex-3-en-1-one O-decyloxime	5.49
		Average	5.49
		Standard Deviation	0.00
Alkyl Carboxylic acid	<chem>C(=O)(O[H])[CX4]</chem>	Butanoic acid	4.90
		Average	4.90
		Standard Deviation	0.00
Aryl Carboxylic acid	<chem>C(=O)(O[H])[c]</chem>	Benzoic acid	4.90
		Average	4.90
		Standard Deviation	0.00

Tertiary amide NN dialkyl	[CX4]C(=O)N([CX4])[CX4]	N-Methylcaprolactam	8.68
		N_N-Diethylacetamide	8.55
		1-Methyl-2-piperidone	8.84
		N_N-Dimethylacetamide	8.48
		N_N-Dicyclohexylacetamide	8.42
		1-methyl-2-pyrrolidone	8.35
		N_N-Dimethylpropionamide	8.31
		N-Acetylpiperidine	8.17
		N_N-Dicyclohexylpropionamide	7.99
		N-Butyrylpiperidine	7.97
		N_N-Diethylnonamide	7.93
		N_N-Dimethylsobutylamide	7.93
		N_N-Diethylbutanamide	7.87
		N_N-Diethylpropanamide	7.71
		N_N-Dimethyltertbutylamide	7.73
		N_N-Dicyclohexyl-2,2-dimethylpropionamide	7.64
		Average	8.16
		Standard Deviation	0.37
Tertiary amide NN diaryl	[CX4]C(=O)N(c)c	N_N-Diphenylacetamide	7.37
		N_N-Diphenylbutanamide	7.08
		N_N-Diphenylpropanamide	6.95
		Average	7.13
		Standard Deviation	0.22
Tertiary Benzamide	[c]C(=O)N([CX4])[CX4]	N_N-Dimethyl-4-methylbenzamide	8.11
		N_N-Dicyclohexylbenzamide	8.02
		N_N-Dimethylbenzamide	8.02
		N-Benzoylpiperidine	7.87
		N_N-Diethylbenzamide	7.83
		Average	7.97
		Standard Deviation	0.03

Secondary alkyl amide	<chem>C(=O)([CX4])N([H])[CX4]</chem>	N-Methylacetamide	8.17
		N-Ethylacetamide	8.15
		N-Methylpropionamide	8.04
		N-Propionylpiperidine	8.00
		Average	8.09
		Standard Deviation	0.08
Secondary benzamide		N-methylbenzamide	7.57
		Average	7.57
		Standard Deviation	0.00
Formamide	<chem>C(=O)([H])N([H])[CX4]</chem>	N,N-Dimethylformamide	7.73
		N,N-Diethylformamide	7.68
		1-Formylpiperidine	7.66
		Average	7.69
		Standard Deviation	0.03
Imide	<chem>N(C(=O)[CX4cCX3])([Cc])C(=O)[CX4cCX3]</chem>	N-Methylsuccinimide	6.08
		N-Methylmaleimide	5.77
		Average	5.93
		Standard Deviation	0.22
NN dialky N'N' dialky tertiary urea	<chem>[CX4]N([CX4])C(=O)N([CX4])[CX4]</chem>	1_1_3_3-tetramethylurea	8.50
		1_1_3_3-tetraethylurea	8.50
		Average	8.50
		Standard Deviation	0.00
N aryl N alkyl N' alkyl N' aryl tertiary urea	<chem>[c]N([CX4])C(=O)N([CX4])[c]</chem>	1_3-diphenyl-1_3-diethylurea	7.90
		Average	7.90

		Standard Deviation	0.00
NN diaryl N'N' dialkyl tertiary urea	<chem>[c]N([c])C(=O)N([CX4])[CX4]</chem>	1_1-diphenyl-3_3-dimethylurea	7.70
		1_1-diphenyl-3_3-diethylurea	7.70
		Average	7.70
		Standard Deviation	0.00
NN diaryl N'N' diaryl tertiary urea	<chem>[c]N([c])C(=O)N([CX4])[CX4]</chem>	1_1_3_3-tetraphenylurea	6.90
		Average	6.90
		Standard Deviation	0.00
Alkyl nitrile	<chem>N#C[CX4]([CX4H])([CX4H])([CX4H])</chem>	isobutylnitrile	5.28
		trimethylacetonitrile	5.26
		propionitrile	5.19
		1-Cyanobutane	5.16
		1-Cyanopentane	5.15
		acetonitrile	5.08
		Average	5.19
		Standard Deviation	0.07
Mono Chloro Nitrile	<chem>N#C[CX4]([Cl])([CX4H])([CX4H])</chem>	Chloroacetonitrile	3.93
		Average	3.93
		Standard Deviation	0.00
Dichloro Nitrile	<chem>N#C[CX4]([Cl])([Cl])([CX4H])</chem>	Dichloroacetonitrile	3.40
		Average	3.40
		Standard Deviation	0.00
Aryl nitrile	<chem>N#CC:1:c(:c(:c(:c(:c:1[CeH]))[CeH])[CeH])[CeH]</chem>	2_6-dimethylbenzonitrile	4.97
		benzonitrile	4.84
		3-Toluonitrile	4.95

		Average	4.92
		Standard Deviation	0.07
Para halogenated aryl nitrile	<chem>N#CC:1:c(:c(:c(:c(:c:1[CcH])[CcH])[FCIBrI])[CcH])[CcH]</chem>	4-fluorobenzonitrille	4.66
		4-Chlorobenzonitrille	4.53
		Average	4.59
		Standard Deviation	0.09
Benzyl nitrile	<chem>N#CC(c:1:c:c:c:c:1)([CX4H])[CX4H]</chem>	Phenylacetoneitrille	4.80
		Average	4.80
		Standard Deviation	0.00
Allyl Nitrile	<chem>N#CC(C=C)([CX4H])[CX4H]</chem>	allylcyanide	4.99
		Average	4.99
		Standard Deviation	0.00
Nitrile C=C	<chem>N#CC=C</chem>	acrylonitrile	4.62
		Average	4.62
		Standard Deviation	0.00
Phenol	<chem>c:1(:c(:c(:c(:c:1[CcH])[CcH])O[H])[CcH])[CcH])[CcH]</chem>	Phenol	2.90
		3-methylphenol	3.10
		4-methylphenol	3.10
		Average	3.02
		Standard Deviation	0.00
Alkyl nitro	<chem>N(=O)(=O)[CX4]</chem>	2-Methyl-2-nitropropane	4.00
		2-Nitropropane	4.00
		Nitroethane	3.80
		Nitromethane	3.70

		Average	3.88
		Standard Deviation	0.15
Aryl nitro	<chem>N(=O)(=O)[c]</chem>	4-Nitrotoluene	3.80
		Nitrobenzene	3.70
		Average	3.75
		Standard Deviation	0.07
Dialkyl sulphoxide	<chem>[SX3](=O)([CX4])[CX4]</chem>	Di-isopropyl sulphoxide	8.75
		Dibutyl sulphoxide	8.71
		Dimethyl sulphoxide	8.60
		Average	8.68
		Standard Deviation	0.08
Alkyl aryl sulphoxide	<chem>[SX3](=O)([c])[CX4]</chem>	(methylsulfinyl)benzene	7.83
		Average	7.83
		Standard Deviation	0.00
Diaryl sulphoxide	<chem>[SX3](=O)([c])[c]</chem>	Di(p-tolyl) sulphoxide	7.77
		Diphenyl sulphoxide	7.48
		Average	7.63
		Standard Deviation	0.20
Secondary cyclic thioamide	<chem>[CR](=S)([cCX4])N([CX4c])[H]</chem>	ϵ -Thiocaprolactam	6.62
		Average	6.62
		Standard Deviation	0.00
Secondary acyclic thioamide	<chem>[CR](=S)([cCX4])N([CX4c])[H]</chem>	N-Methylthioacetamide	5.59
		Average	5.59

		Standard Deviation	0.00
Tertiary thioformamide	[H]C(=S)N([CX4])[CX4]	N_N-dimethylthioformamide	5.40
		Average	5.40
		Standard Deviation	0.00
Tertiary alkyl thioamide	C(=S)([CX4])N([CX4])[CX4]	N_N-dimethylthioacetamide	6.00
		Average	6.00
		Standard Deviation	0.00
Tertiary thiobenzamide	C(=S)(c)N([CX4])[CX4]	4_N_N-trimethylthiobenzamide	5.60
		N_N-dimethylthiobenzamide	5.30
		Average	5.45
		Standard Deviation	0.21
Trialkyl phosphine oxide	P=O([CX4])([CX4])([CX4])	Triethylphosphine oxide	11.10
		Tripropyl oxide	10.80
		Trimethylphosphine oxide	10.70
		Tributylphosphine oxide	10.20
		Average	10.70
		Standard Deviation	0.37
Triaryl phosphine oxide	P=O([c])([c])([c])	Triphenylphosphine oxide	10.10
		Average	10.10
		Standard Deviation	0.00
Phosphine	[PX3]([Cc])([Cc])[cC]	Triphenyl phosphine	5.52
		Average	5.52
		Standard Deviation	0.00

Sulphone alkyl alkyl	<chem>S(=O)(=O)([CX4])([CX4])</chem>	Tetramethylene sulfone	6.30
		Dimethyl sulphone	6.20
		Dibutyl sulphone	6.40
		Average	6.30
		Standard Deviation	0.10
Sulphone aryl aryl	<chem>S(=O)(=O)([c])([c])</chem>	Diphenyl sulphone	5.90
		Average	5.90
		Standard Deviation	0.00
		Dihydro-2(3H)-thiophenone	5.15
Thioester	<chem>C(=O)([cCX4])S[cCX4]</chem>	Average	5.20
		Standard Deviation	0.00
Secondary sulphonamide	<chem>[cC]S(=O)(=O)N([H])([cC])</chem>	N-Methylmethanesulphonamide	5.85
		Average	5.85
		Standard Deviation	0.00
Tertiary sulphonamide NN dialkyl	<chem>S(=O)(=O)([CX4])N([CX4])([CX4])</chem>	N,N-Dimethylmethanesulphonamide	5.95
		Average	5.95
		Standard Deviation	0.00
Tertiary sulphonbenzamide NN dialkyl	<chem>S(=O)(=O)([c])N([CX4])([CX4])</chem>	N,N-Dimethylbenzenesulphonamide	5.71
		Average	5.71
		Standard Deviation	0.00
Tertiary sulphonamide N	<chem>S(=O)(=O)([CX4])N([c])([CX4])</chem>	N-Methyl-N-Benzylsulphonamide	5.22

alkyl N aryl			
		Average	5.22
		Standard Deviation	0.00
Dialkyl thioether	[CX4][SX2][CX4]	Diisopropyl sulphide	3.80
		tert-butyl n-butyl sulphide	3.70
		Sec-butyl n-butyl sulphide	3.60
		Dibutyl sulphide	3.60
		Di(tert-butyl) sulphide	3.60
		Diethyl sulphide	3.60
		Dimethyl sulphide	3.50
		Isobuty n-butyl sulphide	3.50
		Average	3.61
		Standard Deviation	0.10
Tertiary carbamate NN dialky O alkyl	O(C(=O)N([CX4])[CX4])[CX4]	Ethyl diethylcarbamate	7.40
		Ethyl dimethylcarbamate	7.10
		Methyl dimethylcarbamate	7.10
		Average	7.20
		Standard Deviation	0.17
Tertiary carbamate NN diaryl O alkyl	O(C(=O)N([c])[c])[CX4]	Ethyl diphenylcarbamate	6.30
		Methyl diphenylcarbamate	6.20
		Average	6.25
		Standard Deviation	0.07
Tertiary carbamate NN diaryl O aryl	O(C(=O)N([c])[c])[c]	Phenyl diphenylcarbamate	5.70
		Average	5.70
		Standard Deviation	0.00
Thiocyanate	[CX4]SC#N	Methyl thiocyanate	4.68

		Ethyl thiocyanate	4.39
		Average	4.54
		Standard Deviation	0.21
Isothiocyanate	<chem>[cCX4]N=C=S</chem>	Ethyl isothiocyanate	2.92
		Average	2.90
		Standard Deviation	0.00
Pyridine	<chem>[nX2]1cccc1</chem>	2_4_6-Trimethylpyridine	8.10
		3_4-Dimethylpyridine	8.00
		3_5-Dimethylpyridine	8.00
		2_6-Dimethylpyridine	7.80
		4-tert-Butylpyridine	7.70
		4-Methylpyridine	7.70
		4-Ethylpyridine	7.70
		2-Methylpyridine	7.60
		3-Ethylpyridine	7.50
		3-Methylpyridine	7.50
		4-Phenylpyridine	7.40
		4-Isopropylpyridine	7.40
		4-Vinylpyridine	7.40
		2-Ethylpyridine	7.40
		2_4-Dimethylpyridine	7.20
		2-Butylpyridine	7.20
		Pyridine	7.20
		2-Isopropylpyridine	7.00
		2-Vinylpyridine	6.70
		2_6-Diethylpyridine	6.60
		2-Phenylpyridine	6.20
		Average	7.40
		Standard Deviation	0.48
Pyrimidine	<chem>c1([nX2]c([nX2]c(c1[CX4cH])[CX4cH])[CX4cH])[CX4cH]</chem>	4_6-dimethylpyrimidine	6.33
		Pyrimidine	5.44

		Average	5.88
		Standard Deviation	0.63
Triazine	<chem>c:1(:n:c(:n:c(:n:1)[CX4cH])[CX4cH])[CX4cH]</chem>	S-triazine	3.77
		Average	3.77
		Standard Deviation	0.00
Thiourea NN alkyl N' alkyl	<chem>C(=S)(N([CX4])[H])N([CX4])[CX4]</chem>	N-Methyl-N_N'-propylenethiourea	7.51
		Average	7.51
		Standard Deviation	0.00
Thiourea NN dialkyl N'N' dialkyl	<chem>C(=S)(N([CX4])[CX4])N([CX4])[CX4]</chem>	N_N'_N'_N'-Tetramethylthiourea	6.06
		N_N'-Dimethyl-N_N'-ethylenethiourea	5.99
		N_N'-Dimethyl-N'_N'-diethylthiourea	5.93
		Average	5.99
		Standard Deviation	0.07
Furan	<chem>O1C=CC=C1</chem>	Furan	2.20
		Average	2.20
		Standard Deviation	0.00
Thiophene	<chem>S1C=CC=C1</chem>	Thiophene	2.20
		Average	2.20
		Standard Deviation	0.00
Imidazole	<chem>N1(C(=[NX2]C(=C1[CX4Hc])[CX4Hc])[CX4Hc])[H]</chem>	1-methylimidazole	9.06
		4-methylimidazole	8.93
		Imidazole	8.55
		Average	8.85

		Standard Deviation	0.27
Pyrrole	<chem>N1(C(=C(C(=C1[CX4H]))[CX4H]))[CX4H][H]</chem>	Pyrrole	4.12
		1-Methylpyrrole	3.65
		Average	3.88
		Standard Deviation	0.34
Thiazole	<chem>S1C(=C(N=C1[CX4H]))[CX4H][CX4H]</chem>	Thiazole	7.28
		Average	7.28
		Standard Deviation	0.00
Thiazole aryl	<chem>c:1:c2:c(:c:c:c:1)N=CS2</chem>	Benzothiazole	6.06
		Average	6.06
		Standard Deviation	0.00
Isoxazole	<chem>O1N=C(C(=C1[CX4H]))[CX4H][CX4H]</chem>	Isoxazole	4.70
		Average	4.70
		Standard Deviation	0.00
Oxazole	<chem>O1C=CN=C1</chem>	Oxazole	5.77
		Average	5.77
		Standard Deviation	0.00
Pyrazole	<chem>N1=CC=CN1[H]</chem>	1-methylpyrazole	7.15
		Average	7.15
		Standard Deviation	0.00
1,2,3 triazole	<chem>N1=CC=NN1[cC]</chem>	1-Phenylethyl-1_2_3-triazole	7.32
		1-Methylbenzotriazole	6.64
		Average	6.98

		Standard Deviation	0.48
1,3,4 triazole	C1=NC=NN1[cCX4]	1-Butyl-1_3_4-triazole	7.00
		Average	7.00
		Standard Deviation	0.00
1,2,4 triazole	C1=NN=CN1[cCX4]	1-Benzyl-1_2_4-triazole	7.00
		Average	7.00
		Standard Deviation	0.00
Chloride anion	[Cl-1X0]	Tetrabutyl ammonium chloride	12.10
		Average	12.10
		Standard Deviation	0.30 ^a
Bromide anion	[Br-1X0]	Tetraethyl ammonium bromide	10.60
		Tetrabutyl ammonium bromide	10.60
		Tetraoctyl ammonium bromide	10.60
		Average	10.60
		Standard Deviation	0.20 ^a
Iodide anion	[I-1X0]	Tetrabutyl ammonium iodide	8.90
		Tetrahexyl ammonium iodide	9.10
		Average	9.00
		Standard Deviation	0.10 ^a
Hydrogen sulphate anion	S(=[OX1])(=[OX1])([OX1])O([H])	Tetrabutyl ammonium hydrogen sulphate	10.40
		Average	10.40
		Standard Deviation	0.60 ^a
Fluoro alkane	[CX4]F	1-Fluoropentane	2.93
		1-Fluorooctane	3.11
		Fluorocyclohexane	3.26

		Average	3.10
		Standard Deviation	0.17
Chloro alkane	[CX4]Cl	1-Chlorobutane	2.15
		1-Chloropentane	2.22
		2-Chloropropane	2.40
		Chlorocyclohexane	2.46
		1-Chloroadamantane	2.66
		Average	2.38
		Standard Deviation	0.20
Bromo alkane	[CX4]Br	Bromocyclopropane	2.02
		Bromoethane	2.17
		1-Bromopropane	2.22
		1-Bromopentane	2.28
		1-Bromobutane	2.31
		Bromocyclohexane	2.51
		Average	2.25
		Standard Deviation	0.16
Aryl bromide	cBr	Bromobenzene	1.38
		Average	1.38
		Standard Deviation	0.00
Iodo alkane	[CX4]I	Iodomethane	2.02
		Iodoethane	2.02
		1-Iodopentane	2.24
		2-Iodopropane	2.24
		1-Iodoadamantane	2.64
		Average	2.23
		Standard Deviation	0.25
Aryl iodide	cI	Iodobenzene	1.50
		Average	1.50

		Standard Deviation	0.00
Pyrazine	c:1(:c(:c(:c(:n:n:1)[CX4cH])[CX4cH]))[CX4cH])[CX4cH]	2_5-dimethylpyrazine	5.93
		Pyrazine	5.11
		Average	5.52
		Standard Deviation	0.58
Pyridazine	c:1(:c(:n:c(:c(:n:1)[CX4cH])[CX4cH]))[CX4cH])[CX4cH]	Pyridazine	6.73
		Average	6.73
		Standard Deviation	0.00
Pyridine N-oxide	c:1:c:c:[n](c:c:1)[OX1]	Pyridine N-oxide	9.00
		Average	9.00
		Standard Deviation	0.00

^a Standard deviations based on measurements reported in different solvents.