Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# 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 | C([CX4])([CX4])([CX4])O[H] | tert-Butyl alcohol | 2.67 |
| | | tert-Pentanol | 2.65 |
| | | | |
| | | **Average** | 2.66 |
| | | **Standard deviation** | 0.01 |
| | | | |
| Primary aniline | c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])N([H])[H])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N] | β-Naphthylamine | 2.78 |
| | | Aniline | 2.40 |
| | | α-Naphthylamine | 2.60 |
| | | | |
| | | **Average** | 2.62 |
| | | **Standard deviation** | 0.17 |
| | | | |
| | | | |
| Secondary aniline | c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])N([CX4])[H])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N] | N-Methylaniline | 2.06 |
| | | | |
| | | **Average** | 2.06 |
| | | **Standard deviation** | 0.00 |
| | | | |
| Diphenyl aniline | c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])N(c:2:c(:c(:c(:c(:c:2[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[H])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N] | Diphenylaniline | 2.68 |
| | | | |
| | | **Average** | 2.68 |
| | | **Standard deviation** | 0.00 |
| | | | |
| Oxime | N(=C([cCX4])[cCX4])O[H] | 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[CcH])[CcH])O[H])[FClBrI])[CcH])[CcH] | 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])[FClBrI])[CcH1] | 3-Bromophenol | 4.22 |

| | | | |
|---|---|---|---|
| | | 3-Chlorophenol | 4.19 |
| | | 3-Fluorophenol | 4.13 |
| | | | |
| | | **Average** | 4.18 |
| | | **Standard Deviation** | 0.05 |
| | | | |
| Para halogenated phenol | c:1(:c(:c(:c(:c(:c:1[CcH1])[CcH1])O[H])[CcH1])[CcH1])[FClBrI] | 4-Iodophenol | 4.14 |
| | | 4-Bromophenol | 4.11 |
| | | 4-Chlorophenol | 4.10 |
| | | 4-Fluorophenol | 3.93 |
| | | | |
| | | **Average** | 4.07 |
| | | **Standard Deviation** | 0.09 |
| | | | |
| Thiol | [CX4]S[H] | 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 | C(=S)([cCX4])N([CX4c])[H] | Thioacetamide | 3.70 |
| | | Thioacetanilide | 3.40 |
| | | | |
| | | **Average** | 3.55 |
| | | **Standard Deviation** | 0.21 |
| | | | |
| Secondary Sulphonamide | [cC]S(=O)(=O)N([H])([cC]) | N-(2-Naphthyl)toluene-p-sulfonamide | 3.20 |
| | | Touluene-p-sulfonamide | 3.20 |
| | | N-Benzyltoluene-p-sulfonamide | 3.00 |
| | | | |
| | | **Average** | **3.13** |
| | | **Standard Deviation** | **0.12** |
| | | | |
| Thiophenol | c:1:c:c:c(:c:c:1)S[H] | Thiophenol | 1.40 |

| | | | |
|---|---|---|---|
| | | | |
| | | **Average** | **1.40** |
| | | **Standard Deviation** | **0.00** |
| | | | |
| Secondary carbamate N aryl | O(C(=O)N([H])[c])[CX4] | N-Phenylurethane | 2.82 |
| | | | |
| | | **Average** | **2.82** |
| | | **Standard Deviation** | **0.00** |
| | | | |
| Thiourea N alkyl NN alkyl | C(=S)(N([CX4])[H])N([CX4])[CX4] | N-Methyl-N_N'-propylenethiourea | 3.03 |
| | | | |
| | | **Average** | **3.03** |
| | | **Standard Deviation** | **0.00** |
| | | | |
| Pyrrole | N1(C(=C(C(=C1[CX4H])[CX4H])[CX4H])[CX4H])[H] | Pyrrole | 3.02 |
| | | | |
| | | **Average** | **3.03** |
| | | **Standard Deviation** | **0.00** |
| | | | |
| Indole | N1(C=Cc:2c1:c:c:c:c:2)[H] | Indole | 3.14 |
| | | | |
| | | **Average** | **3.14** |
| | | **Standard Deviation** | **0.00** |
| | | | |
| Pyrazole | N1=CC=CN1[H] | 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 | N1=CC=NN1[H] | 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 | C([cC])([cC])([cC])O[H] | Tert-butyl alcohol | 5.70 |
| | | | |
| | | **Average** | 5.70 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| | | | |
| Alkyl alkyl ether | C(OC([!c])([!c])[!c])([!c])([!c])[!c] | 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 | C(OC([!c])([!c])(C=C))([!c])(C=C)[!c] | Diallyl ether | 4.60 |
| | | | |
| | | **Average** | 4.60 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Alkyl aryl ether | cO[CX4] | Anisole | 3.30 |
| | | | |
| | | **Average** | 3.30 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Alkyl alkyl ether benzyl | O(C(C:1:c:c:c:c:c:1)([H])[H])C(C:2:c:c:c:c:c:2)([H])[H] | 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 triflouroacetate | 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 etser | [CX4]C(=O)O[CX4]([CH])([CH])[FClBrI] | Ethyl flouroacetate | 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 | N([H])([CX4!R1]([!c])([!c])[!c])[CX4!R1]([!c])([!c])[!c] | 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 | [NR]([H])([CX4R])([CX4R]) | pyrrolidine | 8.80 |
| | | azetidine | 8.80 |
| | | piperidine | 8.30 |
| | | | |
| | | **Average** | 8.63 |
| | | **Standard Deviation** | 0.29 |
| | | | |
| Dibenzyl secondary amine | N([H])([CX4!R1]([!c])([!c])[c])[CX4!R1]([!c])([!c])[c] | Dibenzylamine | 6.27 |
| | | | |
| | | **Average** | 6.27 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Tetiary amine | N([CX4]([!c])([!c])[!c])([CX4]([!c])([!c])[!c])([CX4]([!c])([!c])[!c]) | 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 | N([CX4]([!c])([!c])C=C)([CX4]([!c])([!c])C=C)([CX4]([!c])([!c])C=C) | Triallylamine | 6.14 |
| | | | |
| | | **Average** | 6.14 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Tribenzyl amine | N([CX4]([!c])([!c])c)([CX4]([!c])([!c])c)([CX4]([!c])([!c])c) | Tribenzylamine | 3.79 |
| | | | |
| | | **Average** | 3.79 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Primary aniline | c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])N([H])[H])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N] | 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 | c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])N([H])[H])[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])[FClBrI] | 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 | c:1(:c(:c(:c(:c(:c:1[!F!Cl!Br!I!O!N])[!F!Cl!Br!I!O!N])N([H])[H])[!F!Cl!Br!I!O!N])[FClBrI])[!F!Cl!Br!I!O!N] | 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] | Benzaldhyde | 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: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 | C(=O)([CX4!R]([!c])([!c])[!c])[CX4!R]([!c])([!c])[!c] | 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 | C(=O)(c:1:c:c:c:c:c:1)c:2:c:c:c:c:c:2 | Benzophenone | 5.44 |
| | | Anthrone | 5.64 |
| | | | |
| | | **Average** | 5.54 |
| | | **Standard Deviation** | 0.14 |
| | | | |
| Dibenzyl ketone | [C!R](=O)([CX4]c)([CX4]c) | Dibenzyl ketone | 5.30 |
| | | | |
| | | **Average** | 5.54 |
| | | **Standard Deviation** | 0.14 |
| | | | |
| Mono halogenated ketone | [C!R](=O)([CX4!R])C(Cl)([CH])[CH] | Chloropropan-2-one | 4.53 |

| | | | |
|---|---|---|---|
| | | | |
| | | **Average** | 4.53 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Tri halogenated ketone | C(=O)([CX4!R])C([FClBrI])([FClBrI])([FClBrI]) | 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 | C1C=CC([CX4]C1)=O | Piperitone | 6.14 |
| | | | |
| | | **Average** | 6.14 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| O aryl substituted Oxime | cON=C([cCX4])([cCX4]) | Acetone O-phenyloxime | 4.77 |
| | | | |
| | | **Average** | 4.77 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| O alkyl substituted Oxime | [CX4]ON=C([cCX4])([cCX4]) | (1E)-Cyclohex-3-en-1-one O-decyloxime | 5.49 |
| | | | |
| | | **Average** | 5.49 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Alkyl Carboxylic acid | C(=O)(O[H])[CX4] | Butanoic acid | 4.90 |
| | | | |
| | | **Average** | 4.90 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Aryl Carboxylic acid | C(=O)(O[H])[c] | 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 | C(=O)([CX4])N([H])[CX4] | 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 | C(=O)([H])N([H])[CX4] | N_N-Dimethylformamide | 7.73 |
| | | N_N-Diethylformamide | 7.68 |
| | | 1-Formylpiperidine | 7.66 |
| | | | |
| | | **Average** | 7.69 |
| | | **Standard Deviation** | 0.03 |
| | | | |
| Imide | N(C(=O)[CX4cCX3])([Cc])C(=O)[CX4cCX3] | N-Methylsuccinimide | 6.08 |
| | | N-Methylmaleimide | 5.77 |
| | | | |
| | | **Average** | 5.93 |
| | | **Standard Deviation** | 0.22 |
| | | | |
| NN dialky N'N' dialky tertiary urea | [CX4]N([CX4])C(=O)N([CX4])[CX4] | 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 | [c]N([CX4])C(=O)N([CX4])[c] | 1_3-diphenyl-1_3-diethylurea | 7.90 |
| | | | |
| | | **Average** | 7.90 |

| | | | |
|---|---|---|---|
| | | **Standard Deviation** | 0.00 |
| | | | |
| NN diaryl N'N' dialkyl tertiary urea | [c]N([c])C(=O)N([CX4])[CX4] | 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 | [c]N([c])C(=O)N([CX4])[CX4] | 1_1_3_3-tetraphenylurea | 6.90 |
| | | | |
| | | **Average** | 6.90 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Alkyl nitrile | N#C[CX4]([CX4H])([CX4H])([CX4H]) | 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 | N#C[CX4]([Cl])([CX4H])([CX4H]) | Chloroacetonitrille | 3.93 |
| | | | |
| | | **Average** | 3.93 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Dichloro Nitrile | N#C[CX4]([Cl])([Cl])([CX4H]) | Dichloroacetonitrille | 3.40 |
| | | | |
| | | **Average** | 3.40 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Aryl nitrile | N#CC:1:c(:c(:c(:c(:c:1[CcH])[CcH])[CcH])[CcH])[CcH] | 2_6-dimethylbenzonitrile | 4.97 |
| | | benzonitrile | 4.84 |
| | | 3-Toluonitrille | 4.95 |

| | | | |
|---|---|---|---|
| | | | |
| | | **Average** | 4.92 |
| | | **Standard Deviation** | 0.07 |
| | | | |
| Para halogenated aryl nitrile | N#CC:1:c(:c(:c(:c(:c:1[CcH])[CcH])[FClBrI])[CcH])[CcH] | 4-fluorobenzonitrille | 4.66 |
| | | 4-Chlorobenzonitrille | 4.53 |
| | | | |
| | | **Average** | 4.59 |
| | | **Standard Deviation** | 0.09 |
| | | | |
| Benzyl nitrile | N#CC(c:1:c:c:c:c:c:1)([CX4H])[CX4H] | Phenylacetonitrille | 4.80 |
| | | | |
| | | **Average** | 4.80 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Allyl Nitrile | N#CC(C=C)([CX4H])[CX4H] | allylcyanide | 4.99 |
| | | | |
| | | **Average** | 4.99 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Nitrile C=C | N#CC=C | acrylonitrile | 4.62 |
| | | | |
| | | **Average** | 4.62 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Phenol | c:1(:c(:c(:c(:c(:c:1[CcH])[CcH])O[H])[CcH])[CcH])[CcH] | Phenol | 2.90 |
| | | 3-methylphenol | 3.10 |
| | | 4-methylphenol | 3.10 |
| | | | |
| | | **Average** | 3.02 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Alkyl nitro | N(=O)(=O)[CX4] | 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 | N(=O)(=O)[c] | 4-Nitrotoluene | 3.80 |
| | | Nitrobenzene | 3.70 |
| | | | |
| | | **Average** | 3.75 |
| | | **Standard Deviation** | 0.07 |
| | | | |
| | | | |
| Dialkyl sulphoxide | [SX3](=O)([CX4])[CX4] | Di-isopropyl sulphoxide | 8.75 |
| | | Dibutyl sulphoxide | 8.71 |
| | | Dimethyl sulphoxide | 8.60 |
| | | | |
| | | **Average** | 8.68 |
| | | **Standard Deviation** | 0.08 |
| | | | |
| Alkyl aryl sulphoxide | [SX3](=O)([c])[CX4] | (methylsulfinyl)benzene | 7.83 |
| | | | |
| | | **Average** | 7.83 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Diaryl sulphoxide | [SX3](=O)([c])[c] | Di(p-tolyl) sulphoxide | 7.77 |
| | | Diphenyl sulphoxide | 7.48 |
| | | | |
| | | **Average** | 7.63 |
| | | **Standard Deviation** | 0.20 |
| | | | |
| | | | |
| Secondary cyclic thioamide | [CR](=S)([cCX4])N([CX4c])[H] | ε-Thiocaprolactam | 6.62 |
| | | | |
| | | **Average** | 6.62 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Secondary acyclic thioamide | [CR](=S)([cCX4])N([CX4c])[H] | 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 phopshine 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 | S(=O)(=O)([CX4])([CX4]) | Tetramethylene sulfone | 6.30 |
| | | Dimethyl sulphone | 6.20 |
| | | Dibutyl sulphone | 6.40 |
| | | | |
| | | | |
| | | **Average** | 6.30 |
| | | **Standard Deviation** | 0.10 |
| | | | |
| Sulphone aryl aryl | S(=O)(=O)([c])([c]) | Diphenyl sulphone | 5.90 |
| | | | |
| | | **Average** | 5.90 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| | | Dihydro-2(3H)-thiophenone | 5.15 |
| | | | |
| Thioester | C(=O)([cCX4])S[cCX4] | **Average** | 5.20 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Secondary sulfonamide | [cC]S(=O)(=O)N([H])([cC]) | N-Methylmethanesulphonamide | 5.85 |
| | | | |
| | | **Average** | 5.85 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Tertiary sulphonamide NN dialkyl | S(=O)(=O)([CX4])N([CX4])([CX4]) | N_N-Dimethylmethanesulphonamide | 5.95 |
| | | | |
| | | **Average** | 5.95 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Tertiary sulphonbenzamide NN dialkyl | S(=O)(=O)([c])N([CX4])([CX4]) | N_N-Dimethylbenzenesulphonamide | 5.71 |
| | | | |
| | | **Average** | 5.71 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Tertairy sulphonamide N | S(=O)(=O)([CX4])N([c])([CX4]) | N-Methyl_N-Benzylsulfonamide | 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 | [cCX4]N=C=S | Ethyl isothiocyanate | 2.92 |
| | | | |
| | | **Average** | 2.90 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Pyridine | [nX2]1ccccc1 | 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 | c1([nX2]c([nX2]c(c1[CX4cH])[CX4cH])[CX4cH])[CX4cH] | 4_6-dimethylpyrimidine | 6.33 |
| | | Pyrimidine | 5.44 |
| | | | |

| | | | |
|---|---|---|---|
| | | | |
| | | **Average** | 5.88 |
| | | **Standard Deviation** | 0.63 |
| | | | |
| Triazine | c:1(:n:c(:n:c(:n:1)[CX4cH])[CX4cH])[CX4cH] | S-triazine | 3.77 |
| | | **Average** | 3.77 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Thiourea NN alkyl N' alkyl | C(=S)(N([CX4])[H])N([CX4])[CX4] | N-Methyl-N_N'-propylenethiourea | 7.51 |
| | | | |
| | | **Average** | 7.51 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Thiourea NN dialkyl N'N' dialkyl | C(=S)(N([CX4])[CX4])N([CX4])[CX4] | 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 | O1C=CC=C1 | Furan | 2.20 |
| | | | |
| | | **Average** | 2.20 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Thiophene | S1C=CC=C1 | Thiophene | 2.20 |
| | | | |
| | | **Average** | 2.20 |
| | | **Standard Deviation** | 0.00 |
| | | | |
| Imidazole | N1(C(=[NX2]C(=C1[CX4Hc])[CX4Hc])[CX4Hc])[H] | 1-methylimidazole | 9.06 |
| | | 4-methylimidazole | 8.93 |
| | | Imidazole | 8.55 |
| | | | |
| | | **Average** | 8.85 |

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