# Electronic Supplementary Information

## p$K_a$ Prediction from an *ab initio* Bond Length: Part 2 – Phenols

## p$K_a$ Prediction from an *ab initio* Bond Length: Part 3 – Benzoic Acids and Anilines

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**Table S1.**

**Identification numbers, experimental p$K_a$ values, SMILES, chemical names and literature references for all compounds.**

| ID | SMILES | Chemical Name | Exp. p$K_a$ | Ref. |
|---|---|---|---|---|
| **Meta/Para- Phenols** | | | | |
| 1 | NCCc1ccc(O)cc1 | 4-(2-aminoethyl)phenol | 9.77 | 1 |
| 2 | Cc1c(Cl)ccc(O)c1 | 3-methyl-4-chlorophenol | 9.20 | 1 |
| 3 | CC(Cc1ccc(O)cc1)(C)C | 4-tert-amylphenol | 10.43 | 1 |
| 4 | c1(cc(O)ccc1[N+](=O)[O-])C(F)(F)F | 3-trifluoromethyl-4-nitrophenol | 6.07 | 1 |
| 5 | c1(Cl)c(C)cc(cc1C)O | 4-chloro-3,5-dimethylphenol | 9.70 | 1 |
| 6 | c1(ccc(cc1)O)c2ccccc2 | 4-phenylphenol | 9.55 | 1 |
| 7 | C(OCCCC)(=O)c1ccc(cc1)O | 4-hydroxy nutyl benzoate | 8.47 | 1 |
| 8 | c1(Cl)c(Cl)ccc(O)c1 | 3,4-dichlorophenol | 8.63 | 1 |
| 9 | c1(C)cc(O)ccc1C | 3,4-dimethylphenol | 10.36 | 1 |
| 10 | C(C)(C)(C)c1ccc(cc1)O | 4-t-butylyphenol | 10.39 | 1 |

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|---|---|---|---|---|
| 11 | C(F)(F)(F)c1cccc(O)c1 | 3-trifluoromethylphenol | 8.95 | 1 |
| 12 | C(C)(=O)c1ccc(cc1)O | 4-hydroxyacetophenone | 8.05 | 1 |
| 13 | c1(C(C)C)ccc(cc1)O | 4-isopropylphenol | 10.24 | 1 |
| 14 | O=Cc1cccc(O)c1 | 3-hydroxybenzaldehyde | 8.98 | 1 |
| 15 | [N+](=O)([O-])c1ccc(cc1)O | 4-nitrophenol | 7.15 | 1 |
| 16 | C(C)(=O)Nc1ccc(cc1)O | n-(4-hydroxyphenyl)acetamide | 9.38 | 1 |
| 17 | c1(ccc(cc1)O)Cl | 4-chlorophenol | 9.41 | 1 |
| 18 | c1(O)ccc(cc1)C | 4-cresol | 10.26 | 1 |
| 19 | c1(ccc(cc1)O)Br | 4-bromophenol | 9.17 | 1 |
| 20 | c1(ccccc1)O | phenol | 9.99 | 1 |
| 21 | c1(O)cc(C)cc(C)c1 | 3,5-dimethylphenol | 10.19 | 1 |
| 22 | c1c(cccc1Cl)O | 3-chlorophenol | 9.12 | 1 |
| 23 | c1c(C)cccc1O | 3-cresol | 10.09 | 1 |
| 24 | C(OCC)(=O)c1ccc(cc1)O | 4-hydroxybenzoic acid, ethyl ester | 8.34 | 1 |
| 25 | c1(cccc(O)c1)C(C)=O | 3-hydroxyacetophenone | 9.25 | 1 |
| 26 | c1(ccc(cc1)O)N | 4-aminophenol | 10.45 | 1 |
| 27 | O=Cc1ccc(cc1)O | 4-hydroxybenzaldehyde | 7.61 | 1 |
| 28 | c1(O)ccc(cc1)CC | 4-ethylphenol | 10.00 | 1 |
| 29 | c1(O)ccc(cc1)OC | 4-methoxyphenol | 10.10 | 1 |
| 30 | c1c(cccc1O)OC | 3-methoxyphenol | 9.65 | 1 |
| 31 | c1(ccc(cc1)O)F | 4-fluorophenol | 9.91 | 1 |
| 32 | c1c(cccc1F)O | 3-fluorophenol | 9.21 | 1 |
| 33 | C(F)(F)(F)c1ccc(cc1)O | 4-trifluoromethylphenol | 8.68 | 1 |
| 34 | c1(O)cc(OC)cc(OC)c1 | 3,5-dimethoxyphenol | 9.34 | 1 |
| 35 | c1(ccc(cc1)O)I | 4-iodophenol | 9.21 | 1 |
| 36 | [N+](=O)([O-])c1cccc(O)c1 | 3-nitrophenol | 8.36 | 1 |
| 37 | c1(cc(O)ccc1[N+](=O)[O-])[N+](=O)[O-] | 3,4-dinitrophenol | 5.42 | 1 |
| 38 | c1(cccc(O)c1)c2ccccc2 | 3-phenylphenol | 9.64 | 1 |
| 39 | c1(cccc(O)c1)C(C)(C)C | 3-(1,1-dimethylethyl)-phenol | 10.12 | 1 |
| 40 | [N+](=O)([O-])c1cc(O)cc(c1)[N+](=O)[O-] | 3,5-dinitrophenol | 6.69 | 1 |

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|---|---|---|---|---|
| 41 | c1(Cl)cc(O)cc(Cl)c1 | 3,5-dichlorophenol | 8.18 | 1 |
| 42 | c1c(cccc1N)O | 3-aminophenol | 9.86 | 1 |
| 43 | c1c(cccc1Br)O | 3-bromophenol | 9.03 | 1 |
| 44 | c1(Cl)c(Cl)cc(cc1Cl)O | 3,4,5-trichlorophenol | 7.84 | 1 |
| 45 | c1(cccc(O)c1)C(C)C | 3-isopropylphenol | 10.16 | 1 |
| 46 | c1c(CC)cccc1O | 3-ethylphenol | 9.90 | 1 |
| 47 | c1c(cccc1O)OCC | 3-ethoxyphenol | 9.65 | 1 |
| 48 | c1(O)ccc(cc1)OCC | 4-ethoxyphenol | 10.13 | 1 |
| 49 | c1(Br)cc(O)cc(Br)c1 | 3,5-dibromophenol | 8.06 | 1 |
| 50 | c1c(cccc1I)O | 3-iodophenol | 9.03 | 1 |
| 51 | c1(O)ccc(cc1)CCC | 4-propylphenol | 10.34 | 1 |
| 52 | c1(O)cc(CC)cc(C)c1 | 3-ethyl-5-methylphenol | 10.10 | 1 |
| 53 | N#Cc1ccc(cc1)O | 4-cyanophenol | 7.97 | 1 |
| 54 | N#Cc1cccc(O)c1 | 3-cyanophenol | 8.61 | 1 |
| 55 | c1(O)ccc(cc1)CS | 4-methiophenol | 9.53 | 1 |
| 56 | c12CCCc1ccc(O)c2 | 5-indanol | 10.32 | 1 |
| 57 | [N+](=O)([O-])c1c(C)ccc(O)c1 | 3-nitro-4-cresol | 8.62 | 1 |
| 58 | C(C)(=O)c1ccc(cc1)O | hydroxyacetophenone | 8.05 | 1 |
| | | | | |
| **Ortho- Phenols (Capable of forming internal hydrogen bonds)** | | | | |
| 59 | c1(ccccc1O)C(N)=O | 2-hydroxybenzamide | 8.89 | 1 |
| 60 | C(=O)(Nc1ccccc1)c2ccccc2O | salicylanilide | 7.40 | 1 |
| 61 | c1(ccccc1O)C(OC)=O | methyl salicylate | 9.87 | 1 |
| 62 | c1(O)c(cccc1C=O)OC | 2-vanillin | 7.91 | 1 |
| 63 | c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(cc2)Cl | 3,5,4'-trichloro salicylanilide | 4.70 | 1 |
| 64 | C(=O)(Nc1ccccc1Cl)c2ccccc2O | 2'-chloro salicylanilide | 7.31 | 1 |
| 65 | c1(c(O)ccc(c1)N(=O)=O)C(=O)Nc2ccccc2 | 5-nitro salicylanilide | 3.03 | 1 |
| 66 | C(=O)(Nc1ccc(cc1)Br)c2ccccc2O | 4'-bromo salicylanilide | 7.31 | 1 |
| 67 | c1(cc(ccc1O)Br)C(=O)Nc2ccc(cc2)Cl | 4'-chloro-5-bromo salicylanilide | 6.00 | 1 |
| 68 | C(=O)(Nc1ccc(cc1)Cl)c2ccccc2O | 4'-chloro salicylanilide | 7.30 | 1 |

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|---|---|---|---|---|
| 69 | c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccccc2 | 3,5-dichloro salicylanilide | 4.70 | 1 |
| 70 | c1(cc(ccc1O)Cl)C(=O)Nc2ccccc2 | 5-chlorosalicylanilide | 6.17 | 1 |
| 71 | c1(cc(ccc1O)Cl)C(=O)Nc2ccccc2C | 5-chloro-2'-methyl salicylanilide | 6.60 | 1 |
| 72 | C(=O)(Nc1ccc(Cl)cc1Cl)c2ccccc2O | 2',4'-dichloro salicylanilide | 7.14 | 1 |
| 73 | N(=O)(=O)c1ccccc1NC(=O)c2ccccc2O | 2'-nitro salicylanilide | 6.91 | 1 |
| 74 | c1(cc(ccc1NC(=O)c2ccccc2O)Cl)N(=O)=O | 2'-nitro-4'-chloro salicylanilide | 6.74 | 1 |
| 75 | c1(ccc(Br)c(C)c1O)C(NC)=O | 5-bromo-2-hydroxy-n,3-dimethyl-benzamide | 7.52 | 1 |
| 76 | c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(cc2)F | 3,5-dichloro-4'-fluoro salicylanilide | 4.80 | 1 |
| 77 | c1(cc(cc(Br)c1O)Br)C(=O)Nc2ccc(Cl)cc2N(=O)=O | 3,5-dibromo-2'-nitro-4'-chloro salicylanilide | 4.11 | 1 |
| 78 | C(=O)(Nc1ccc(Cl)cc1C)c2ccccc2O | 2'-methyl-4'-chloro salicylanilide | 7.43 | 1 |
| 79 | c1(cc(ccc1O)F)C(=O)Nc2ccc(Br)cc2C | 5-fluoro-2'-methyl-4'-bromo salicylanilide | 7.10 | 1 |
| 80 | c1(cc(ccc1O)F)C(=O)Nc2ccc(Cl)cc2C | 5-fluoro-2'-methyl-4'-chloro salicylanilide | 7.30 | 1 |
| 81 | c1(cc(cc(Br)c1O)Br)C(=O)Nc2ccc(F)cc2F | 3,5-dibromo-2',4'-difluoro salicylanilide | 4.77 | 1 |
| 82 | c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(F)cc2F | 3,5-dichloro-2',4'-difluoro salicylanilide | 4.77 | 1 |
| 83 | c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(Cl)cc2N(=O)=O | 3,5,-4'-trichloro-2'-nitro salicylanilide | 4.11 | 1 |
| 84 | c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(cc2C)N(=O)=O | 3,5-dichloro-2'-methyl-4'-nitro salicylanilide | 4.41 | 1 |
| | | | | |
| **Ortho- Phenols** | | | | |
| 85 | c1(c(O)ccc(c1)[N+](=O)[O-])[N+](=O)[O-] | 2,4-dinitrophenol | 4.09 | 1 |
| 86 | c1(Cl)c(O)c(Cl)cc(Cl)c1Cl | 2,3,4,6-tetrachlorophenol | 5.22 | 1 |
| 87 | c1(c(cccc1N(=O)=O)O)N(=O)=O | 2,3-dinitrophenol | 4.96 | 1 |
| 88 | c1(Cl)c(Cl)c(O)c(c(Cl)c1Cl)Cl | pentachlorophenol | 4.70 | 1 |
| 89 | c1(O)c(cccc1Cl)Cl | 2,6-dichlorophenol | 6.79 | 1 |
| 90 | c1(O)c(C)cccc1Cl | 2-methyl-6-chlorophenol | 8.69 | 1 |
| 91 | c1(cc(cc([N+](=O)[O-])c1O)[N+](=O)[O-])[N+](=O)[O-] | 2,4,6-trinitrophenol | 0.38 | 1 |
| 92 | c1(cc(Cl)cc([N+](=O)[O-])c1O)[N+](=O)[O-] | 4-chloro-2,6-dinitrophenol | 2.96 | 1 |
| 93 | c1(cc(cc(C(C)CC)c1O)[N+](=O)[O-])[N+](=O)[O-] | 2-sec-butyl-4,6-dinitrophenol | 4.62 | 1 |
| 94 | [N+](=O)([O-])c1ccccc1O | 2-nitrophenol | 7.23 | 1 |
| 95 | c1(ccccc1O)C(C)C | 2-isopropylphenol | 10.47 | 1 |
| 96 | c1(ccccc1O)C(C)(C)C | 2-t-butylphenol | 10.28 | 1 |

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|---|---|---|---|---|
| 97 | c1(O)c(Cl)cc(cc1Cl)Cl | 2,4,6-trichlorophenol | 6.23 | 1 |
| 98 | c1(O)cc(C)ccc1C(C)C | thymol | 10.62 | 1 |
| 99 | c1(C(C)C)c(O)cc(c(Cl)c1)C | chlorothymol | 9.98 | 1 |
| 100 | [N+](=O)([O-])c1c(O)ccc(Cl)c1 | 4-chloro-2-nitrophenol | 6.46 | 1 |
| 101 | c1(ccccc1O)c2ccccc2 | 2-phenylphenol | 9.92 | 1 |
| 102 | c1(ccccc1OC)O | 2-methoxyphenol | 9.98 | 1 |
| 103 | c1(ccccc1CC)O | 2-ethylphenol | 10.20 | 1 |
| 104 | c1(OC)cc(C)ccc1O | 4-methyl-2-methoxyphenol | 10.28 | 1 |
| 105 | c1(ccccc1OCC)O | 2-ethoxyphenol | 10.11 | 1 |
| 106 | c1c(Cl)c(O)cc(Cl)c1Cl | 2,4,5-trichlorophenol | 7.40 | 1 |
| 107 | c1(O)cc(C)ccc1C | 2,5-dimethylphenol | 10.41 | 1 |
| 108 | c1(ccccc1O)Cl | 2-chlorophenol | 8.56 | 1 |
| 109 | c1(ccccc1O)Br | 2-bromophenol | 8.45 | 1 |
| 110 | c1(ccccc1O)N | 2-aminophenol | 9.75 | 1 |
| 111 | c1(ccccc1C)O | 2-cresol | 10.28 | 1 |
| 112 | c1(c(O)ccc(C(C)(C)C)c1)C(C)(C)C | 2,4-di-t-butylphenol | 11.72 | 1 |
| 113 | c1(OC)cc(ccc1O)C=CC | 2-methoxy-4-(1-propenyl)phenol | 9.88 | 1 |
| 114 | c1(OC)cc(CC=C)ccc1O | eugenol | 10.19 | 1 |
| 115 | c1(ccc(c(Cl)c1)O)C(C)(C)C | 4-(tert-butyl)-2-chlorophenol | 8.58 | 1 |
| 116 | c1(ccc(c(C)c1)O)C(C)(C)C | 4-(t-butyl)-2-cresol | 10.59 | 1 |
| 117 | [N+](=O)([O-])c1ccc(c(N)c1)O | 2-amino-4-nitrophenol | 7.60 | 1 |
| 118 | [N+](=O)([O-])c1cc(Br)c(c(Br)c1)O | 2,6-dibromo-4-nitrophenol | 3.39 | 1 |
| 119 | c1(C)cc(C)ccc1O | 2,4-dimethylphenol | 10.60 | 1 |
| 120 | c1(O)c(Br)cc(cc1Br)Br | 2,4,6-tribromophenol | 6.10 | 1 |
| 121 | N(=O)(=O)c1c(O)ccc(N)c1 | phenol, 4-amino-2-nitro- | 7.81 | 1 |
| 122 | [N+](=O)([O-])c1cc(C)ccc1O | 4-methyl-2-nitrophenol | 7.40 | 1 |
| 123 | c1(Cl)c(O)ccc(Cl)c1 | 2,4-dichlorophenol | 7.89 | 1 |
| 124 | c1(OC)cc(ccc1O)C=O | vanillin | 7.40 | 1 |
| 125 | c1(O)c(cccc1C(C)(C)C)C(C)(C)C | 2,6-di-t-butylphenol | 11.70 | 1 |
| 126 | c1(O)c(cc(cc1C(C)(C)C)C)C(C)(C)C | 2,6-di-t-butyl-4-methylphenol (bht) | 12.23 | 1 |

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|---|---|---|---|---|
| 127 | c2(cc(cc(C1CCCCC1)c2O)[N+](=O)[O-])[N+](=O)[O-] | 2-cyclohexyl-4,6-dinitrophenol | 4.52 | 1 |
| 128 | [N+](=O)([O-])c1ccc(cc1O)[N+](=O)[O-] | 2,5-dinitrophenol | 5.21 | 1 |
| 129 | c1(ccccc1O)F | 2-fluorophenol | 8.70 | 1 |
| 130 | [N+](=O)([O-])c1ccc(cc1O)F | 5-fluoro-2-nitrophenol | 6.07 | 1 |
| 131 | c1(O)c(C)cc(c(C)c1)C | 2,4,5-trimethylphenol | 10.57 | 1 |
| 132 | c1(C)c(C)cccc1O | 2,3-dimethylphenol | 10.54 | 1 |
| 133 | c1(O)c(C)cc(cc1C)C | 2,4,6-trimethylphenol | 10.86 | 1 |
| 134 | c1(ccccc1O)I | 2-iodophenol | 8.51 | 1 |
| 135 | c1(c(O)c(C)cc(c1)[N+](=O)[O-])[N+](=O)[O-] | 4,6-dinitro-o-cresol | 4.31 | 1 |
| 136 | c1(O)c(O)ccc(CCN)c1C | 2-methyldopamine= | 9.54 | 1 |
| 137 | [N+](=O)([O-])c1cccc(c1O)[N+](=O)[O-] | 2,6-dinitrophenol | 3.97 | 1 |
| 138 | c1(O)c(C)cccc1C | 2,6-dimethylphenol | 10.62 | 1 |
| 139 | c1(Cl)c(cccc1Cl)O | 2,3-dichlorophenol | 7.70 | 1 |
| 140 | c1(O)c(Cl)ccc(Cl)c1 | 2,5-dichlorophenol | 7.51 | 1 |
| 141 | [N+](=O)([O-])c1cccc(Cl)c1O | 6-chloro-2-nitrophenol | 5.48 | 1 |
| 142 | c1(Br)c(Br)c(O)c(c(Br)c1Br)Br | pentabromophenol | 4.62 | 1 |
| 143 | c1(O)c(cccc1Br)Br | 2,6-dibromophenol | 6.67 | 1 |
| 144 | c1(cc(C)cc([N+](=O)[O-])c1O)[N+](=O)[O-] | 2,6-dinitro-p-cresol | 4.23 | 1 |
| 145 | N#Cc1ccccc1O | 2-cyanophenol | 6.86 | 1 |
| 146 | [N+](=O)([O-])c1ccc(cc1O)Cl | 5-chloro-2-nitrophenol | 6.05 | 1 |
| 147 | c1(Br)c(O)ccc(Br)c1 | 2,4-dibromophenol | 7.79 | 1 |
| 148 | [N+](=O)([O-])c1cc(Cl)c(c(Cl)c1)O | 2,6-dichloro-4-nitrophenol | 3.55 | 1 |
| 149 | [N+](=O)([O-])c1ccc(c(Cl)c1)O | 2-chloro-4-nitrophenol | 5.45 | 1 |
| 150 | c1(O)cc(ccc1OC)C=O | isovanillin | 8.89 | 1 |
| 151 | c1(ccccc1CCC)O | 2-propylphenol | 10.47 | 1 |
| 152 | c1(O)cc(C)cc(C)c1C | 2,3,5-trimethylphenol | 10.67 | 1 |
| 153 | c1(C)cc(c([N+]([O-])=O)cc1)O | 5-methyl-2-nitrophenol | 7.41 | 1 |
| 154 | c2(cc(cc(c1ccccc1)c2O)[N+](=O)[O-])[N+](=O)[O-] | 2,4-dinitro-6-phenylphenol | 3.85 | 1 |
| 155 | c1(C(C)(C)C)cc(C(C)(C)C)cc(C(C)(C)C)c1O | 2,4,6-tri(tert-butyl)phenol | 12.19 | 1 |
| 156 | c1(F)c(F)c(O)c(c(F)c1F)F | pentafluorophenol | 5.53 | 1 |

| | | | | |
|---|---|---|---|---|
| 157 | [N+](=O)([O-])c2c(O)ccc(c1ccccc1)c2 | 4-phenyl-2-nitrophenol | 6.73 | 1 |
| 158 | c1(Cl)c(Cl)ccc(Cl)c1O | 2,3,6-trichlorophenol | 5.80 | 1 |
| 159 | c1(O)c(Cl)c(Cl)cc(Cl)c1Cl | 2,3,5,6-tetrachlorophenol | 5.14 | 1 |
| 160 | c1(cc(cc(Cl)c1O)[N+](=O)[O-])[N+](=O)[O-] | 6-chloro-2,4-dinitrophenol | 2.10 | 1 |
| 161 | [N+](=O)([O-])c1c(O)ccc(OC)c1 | 4-methoxy-2-nitrophenol | 7.31 | 1 |
| 162 | c1(C)cc(Cl)ccc1O | 2-methyl-4-chlorophenol | 9.71 | 1 |
| 163 | c1(O)c(Br)cc(cc1Br)C#N | bromoxynil | 3.86 | 1 |
| 164 | c1(cc(C)cc(C)c1O)C(C)(C)C | 2-(1,1-dimethylethyl)-4,6-dimethylphenol | 12.04 | 1 |
| 165 | c1(O)c(cccc1C(C)C)C(C)C | phenol, 2,6-bis(1-methylethyl)- | 11.10 | 1 |
| 166 | c1(cc(C)ccc1O)C(C)(C)C | 2-(tert-butyl)-4-methylphenol | 11.72 | 1 |
| 167 | [N+](=O)([O-])c1cc(C)c(c(C)c1)O | 2,6-dimethyl-4-nitrophenol | 7.07 | 1 |
| 168 | c1(O)c(Cl)cc(cc1Cl)C | 4-methyl-2,6-dichlorophenol | 7.19 | 1 |
| 169 | c1(O)c(Cl)cc(cc1Cl)Br | 4-bromo-2,6-dichlorophenol | 6.21 | 1 |
| 170 | [N+](=O)([O-])c1c(O)ccc(C(C)CC)c1 | 4-(sec-butyl)-2-nitrophenol | 7.59 | 1 |
| 171 | C(O)(=O)c1ccc(O)c(Cl)c1 | 3-chloro-4-hydroxybenzoic acid | 7.52 | 1 |
| 172 | c1(Cl)c(Cl)c(O)cc(Cl)c1Cl | 2,3,4,5-tetrachlorophenol | 6.35 | 1 |
| 173 | N(=O)(=O)c1ccc(c(O)c1)C | phenol, 2-methyl-5-nitro- | 8.59 | 1 |
| 174 | Cl-c(cc(c1)C)c(c1)O | 2-chloro-4-methylphenol | 8.74 | 1 |
| 175 | c2(c(ON=Cc1cc(Br)c(c(Br)c1)O)ccc(c2)N(=O)=O)N(=O)=O | bromofenoxim | 5.46 | 1 |
| **Meta-/Para-Benzoic Acids** | | | | |
| 176 | C(O)(=O)c1ccc(c(Cl)c1)Cl | 3,4-dichlorobenzoic acid | 3.64 | 1 |
| 177 | c1(cc(Cl)cc(Cl)c1)C(O)=O | 3,5-dichlorobenzoic acid | 3.54 | 1 |
| 178 | S(=O)(=O)(N(CCC)CCC)c1ccc(cc1)C(O)=O | probenecid | 3.40 | 1 |
| 179 | [N+](=O)([O-])c1ccc(cc1)C(O)=O | p-nitrobenzoicacid | 3.44 | 1 |
| 180 | C(O)(c1ccccc1)=O | benzoic acid | 4.19 | 1 |
| 181 | C(O)(=O)c1ccc(cc1)Cl | 4-chlorobenzoic acid | 3.98 | 1 |
| 182 | C(O)(=O)c2ccc1c(cccc1)c2 | 2-naphthoic acid | 4.17 | 1 |
| 183 | C(O)(=O)c1ccc(c(OC)c1)OC | 3,4-dimethoxybenzoic acid | 4.36 | 1 |
| 184 | C(O)(=O)c1ccc(cc1)C(C)(C)C | 4-(tert-butyl)-benzoic acid | 4.40 | 1 |

| | | | | |
|---|---|---|---|---|
| 185 | C(O)(=O)c1ccc(cc1)O | p-hydroxybenzoic acid | 4.54 | 1 |
| 186 | C(O)(=O)c1ccc(cc1)C | p-toluic acid | 4.37 | 1 |
| 187 | C(O)(=O)c1ccc(c(O)c1)O | 3,4-dihydroxybenzoic acid | 4.48 | 1 |
| 188 | [N+](=O)([O-])c1cc(cc(c1)[N+](=O)[O-])C(O)=O | 3,5-dinitrobenzoic acid | 2.82 | 1 |
| 189 | c1(cc(O)cc(O)c1)C(O)=O | 3,5-dihydroxybenzoic acid | 4.04 | 1 |
| 190 | C(O)(=O)c1cccc(N)c1 | 3-aminobenzoic acid | 4.74 | 1 |
| 191 | C(O)(=O)c1cccc(C)c1 | m-toluic acid | 4.27 | 1 |
| 192 | C(O)(=O)c1ccc(cc1)OC | p-methoxybenzoic acid | 4.47 | 1 |
| 193 | [N+](=O)([O-])c1cccc(c1)C(O)=O | m-nitrobenzoic acid | 3.46 | 1 |
| 194 | C(O)(=O)c1ccc(c(OC)c1)O | 4-hydroxy-3-methoxybenzoic acid | 4.51 | 1 |
| 195 | c1(O)c(O)cc(cc1O)C(O)=O | 3,4,5-trihydroxybenzoic acid | 4.21 | 1 |
| 196 | C(O)(=O)c1ccc(cc1)N | 4-aminobenzoic acid | 4.85 | 1 |
| 197 | C(O)(=O)c1cccc(F)c1 | m-fluorobenzoic acid | 3.86 | 1 |
| 198 | C(O)(=O)c1ccc(cc1)F | p-fluorobenzoic acid | 4.14 | 1 |
| 199 | c1(cc(ccc1[N+](=O)[O-])C(O)=O)[N+](=O)[O-] | 3,4-dinitrobenzoic acid | 2.82 | 1 |
| 200 | c1(O)c(OC)cc(cc1OC)C(O)=O | 4-hydroxy-3,5-dimethoxybenzioc acid | 4.34 | 1 |
| 201 | C(O)(=O)c1cccc(Cl)c1 | m-chlorobenzoic acid | 3.81 | 1 |
| 202 | C(O)(=O)c1ccc(cc1)C(C)C | cumic acid | 4.35 | 1 |
| 203 | C(O)(=O)c1cccc(Br)c1 | m-bromobenzoic acid | 3.81 | 1 |
| 204 | C(O)(=O)c1ccc(cc1)C(C)=O | p-acetylbenzoic acid | 3.70 | 1 |
| 205 | C(O)(=O)c1ccc(cc1)Br | p-bromobenzoic acid | 4.00 | 1 |
| 206 | C(O)(=O)c1cccc(OC)c1 | m-methoxybenzoic acid | 4.09 | 1 |
| 207 | C(O)(=O)c1cccc(I)c1 | 3-iodobenzoic acid | 3.85 | 1 |
| 208 | C(O)(=O)c1ccc(cc1)OCC | p-ethoxybenzoic acid | 4.45 | 1 |
| 209 | c(cc(c1)C(=O)O)c(c1)C=O | 4-formylbenzoic acid | 3.77 | 1 |
| 210 | N#Cc1ccc(cc1)C(O)=O | p-cyanobenzoic acid | 3.55 | 1 |
| 211 | C(O)(=O)c1ccc(cc1)CC | 4-ethylbenzoic acid | 4.35 | 1 |
| 212 | C(O)(=O)c1ccc(cc1)I | 4-iodobenzoic acid | 4.00 | 1 |
| 213 | C(O)(=O)c1cccc(c1)C=O | 3-formylbenzoic acid | 3.84 | 1 |
| 214 | Nc1ccc(cc1N)C(O)=O | 3,4-diamino-benzoic acid | 3.49 | 1 |

| | | | | |
|---|---|---|---|---|
| 215 | c1(cc(OC)cc(OC)c1)C(O)=O | 3,5-dimethoxybenzoic acid | 3.97 | 1 |
| 216 | C(O)(=O)c1cccc(c1)C#N | m-cyanobenzoic acid | 3.60 | 1 |
| 217 | C(O)(=O)c1ccc(cc1)Oc2ccccc2 | p-phenoxybenzoic acid | 4.52 | 1 |
| 218 | C(O)(=O)c2cccc(Oc1ccccc1)c2 | m-phenoxybenzoic acid | 3.92 | 1 |
| 219 | S(C)(=O)(=O)c1ccc(cc1)C(O)=O | p-methylsulfonylbenzoic acid | 3.64 | 1 |
| 220 | C(O)(=O)c1ccc(cc1)OCCC | 4-propoxybenzoic acid | 4.46 | 1 |
| 221 | O=C(O)c(cccc1O)c1 | 4-[(acetylamino)amino]-benzoic acid | 4.20 | 1 |
| | | | | |
| **Ortho- Benzoic Acids** | | | | |
| 222 | c1(ccc(cc1O)C)C(O)=O | 4-methylsalicylic acid | 3.40 | 1 |
| 223 | c1(ccc(cc1Cl)Cl)C(O)=O | 2,4-dichlorobenzoic acid | 2.68 | 1 |
| 224 | c1(cc(Cl)ccc1Cl)C(O)=O | 2,5-dichlorobenzoic acid | 2.47 | 1 |
| 225 | c1(ccccc1OC(C)=O)C(O)=O | acetylsalicylic acid | 3.49 | 1 |
| 226 | c1(c(Cl)ccc(Cl)c1Cl)C(O)=O | 2,3,6-trichlorobenzoic acid | 1.50 | 1 |
| 227 | c1(c(cccc1Cl)Cl)C(O)=O | 2,6-dichlorobenzoic acid | 1.59 | 1 |
| 228 | c1(ccc(cc1OCC)N)C(O)=O | 2-ethoxy-4-aminobenzoic acid | 5.09 | 1 |
| 229 | c1(ccccc1Nc2cccc(C)c2C)C(O)=O | mefenamic acid | 4.20 | 1 |
| 230 | c1(ccc(cc1O)N)C(O)=O | p-aminosalicylic acid | 3.66 | 1 |
| 231 | c1(ccccc1O)C(O)=O | salicylic acid | 2.97 | 1 |
| 232 | c1(cccc(C)c1O)C(O)=O | 3-methylsalicylic acid | 2.95 | 1 |
| 233 | c1(ccccc1I)C(O)=O | 2-iodobenzoic acid | 2.93 | 1 |
| 234 | c1(ccccc1Br)C(O)=O | o-bromobenzoic acid | 2.88 | 1 |
| 235 | c1(ccc(cc1O)O)C(O)=O | 2,4-dihydroxybenzoic acid | 3.11 | 1 |
| 236 | c1(cc(C)ccc1O)C(O)=O | 5-methylsalicylic acid | 3.15 | 1 |
| 237 | O=C(O)c(c(O)ccc1Br)c1 | 5-bromosalicylic acid | 2.66 | 1 |
| 238 | c1(ccccc1NC(C)=O)C(O)=O | n-acetyl-o-aminobenzoic acid | 3.40 | 1 |
| 239 | c1(ccc(cc1OC)OC)C(O)=O | 2,4-dimethoxybenzoic acid | 4.36 | 1 |
| 240 | c1(ccccc1Nc2ccccc2)C(O)=O | n-phenyl-o-aminobenzoic acid | 3.99 | 1 |
| 241 | c2(C(O)=O)c(O)cc1ccccc1c2 | 2-naphthalenecarboxylic acid, 3-hydroxy- | 2.79 | 1 |
| 242 | [N+](=O)([O-])c1ccc(c(C(O)=O)c1)O | 5-nitrosalicylic acid | 2.12 | 1 |

| | | | | |
|---|---|---|---|---|
| 243 | [N+](=O)([O-])c1ccc(c(Cl)c1)C(O)=O | 2-chloro-4-nitro-benzoic acid | 2.14 | 1 |
| 244 | c1(ccccc1N)C(O)=O | 2-aminobenzoic acid | 4.95 | 1 |
| 245 | c1(ccccc1Cl)C(O)=O | 2-chlorobenzoic acid | 2.89 | 1 |
| 246 | C(O)(=O)c1ccccc1C | o-toluic acid | 3.98 | 1 |
| 247 | c1(cc(I)ccc1O)C(O)=O | 2-hydroxy-5-iodo-benzoic acid | 2.62 | 1 |
| 248 | c1(C(O)=O)c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-] | 2,4,6-trinitrobenzoic acid | 0.65 | 1 |
| 249 | c1(cc(I)cc(I)c1O)C(O)=O | 3,5-diiodosalicylic acid | 2.30 | 1 |
| 250 | c1(cc(Cl)cc(N)c1Cl)C(O)=O | 3-amino-2,5-dichlorobenzoic acid | 3.40 | 1 |
| 251 | c1(cccc(O)c1O)C(O)=O | 2,3-dihydroxybenzoic acid | 2.91 | 1 |
| 252 | c1(c(cccc1O)O)C(O)=O | 2,6-dihydroxybenzoic acid | 1.05 | 1 |
| 253 | c1(cc(Cl)ccc1O)C(O)=O | 5-chlorosalicylic acid | 2.65 | 1 |
| 254 | c1(ccccc1F)C(O)=O | 2-fluorobenzoic acid | 3.27 | 1 |
| 255 | c1(cc(O)ccc1O)C(O)=O | 2,5-dihydroxybenzoic acid | 2.95 | 1 |
| 256 | [N+](=O)([O-])c1ccccc1C(O)=O | 2-nitrobenzoic acid | 2.17 | 1 |
| 257 | c1(ccccc1C(C)=O)C(O)=O | o-acetylbenzoic acid | 4.13 | 1 |
| 258 | c1(ccccc1OC)C(O)=O | o-methoxybenzoic acid | 3.90 | 1 |
| 259 | c1(cc(cc(C(O)=O)c1O)N(=O)=O)N(=O)=O | 2-hydroxy-3,5-dinitro-benzoic acid | 0.70 | 1 |
| 260 | c1(cc(ccc1C(O)=O)[N+](=O)[O-])[N+](=O)[O-] | 2,4-dinitrobenzoic acid | 1.42 | 1 |
| 261 | C(O)(=O)c1c(C)cccc1C | 2,6-dimethylbenzoic acid | 3.35 | 1 |
| 262 | c1(C(O)=O)c(F)c(F)c(c(F)c1F)C | 2,3,5,6-tetrafluoro-4-methyl-benzoic acid | 2.00 | 1 |
| 263 | c1(ccccc1c2ccccc2)C(O)=O | [1,1-biphenyl]-2-carboxylic acid | 3.46 | 1 |
| 264 | c1(c(cccc1OC)OC)C(O)=O | 2,6-dimethoxybenzoic acid | 3.44 | 1 |
| 265 | c1(cccc(OC)c1OC)C(O)=O | 2,3-dimethoxybenzoic acid | 3.98 | 1 |
| 266 | c1(c(Cl)ccc(Cl)c1OC)C(O)=O | 3,6-dichloro-2-methoxybenzoic acid | 1.97 | 1 |
| 267 | c1(ccccc1Oc2ccccc2)C(O)=O | o-phenoxybenzoic acid | 3.53 | 1 |
| 268 | c1(ccccc1C(C)C)C(O)=O | o-isopropylbenzoic acid | 3.63 | 1 |
| 269 | [N+](=O)([O-])c1ccc(c(C(O)=O)c1)Cl | 2-chloro-5-nitrobenzoic acid | 2.17 | 1 |
| 270 | [N+](=O)([O-])c1cccc(C(O)=O)c1Cl | 2-chloro-3-nitrobenzoic acid | 2.02 | 1 |
| 271 | c2c(NC(c1c(C(O)=O)cccc1)=O)cccc2 | n-phenylphthalamic acid | 2.50 | 1 |
| 272 | N(=O)(=O)c1cccc(Cl)c1C(O)=O | 2-chloro-6-nitro-benzoic acid | 1.34 | 1 |

| | | | | |
|---|---|---|---|---|
| 273 | c1(c(C)cccc1Cl)C(O)=O | 2-chloro-6-methyl-benzoic acid | 2.75 | 1 |
| 274 | c1(ccccc1NCC(N)=O)C(O)=O | 2-[(acetylamino)amino]-benzoic acid | 4.20 | 1 |
| | | | | |
| **Anilines** | | | | |
| 275 | Nc1cc(C(O)=O)ccc1 | 3-aminobenzoic acid | 4.53 | 3 |
| 276 | Nc1ccc(C(O)=O)cc1 | 4-aminobenzoic acid | 2.38 | 2 |
| 277 | Nc1cc(O)c(C(O)=O)cc1 | p-aminosalicylic acid | 2.05 | 2 |
| 278 | Nc1ccc(O)cc1 | 4-amino-phenol | 5.48 | 2 |
| 279 | Nc1cc(O)ccc1 | 3-amino-phenol | 4.37 | 2 |
| 280 | Nc1cc(N(=O)=O)cc(N(=O)=O)c1 | 3,5-dinitroaniline | 0.30 | 2 |
| 281 | Nc1cc(Cl)cc(Cl)c1 | 3,5-dichloroaniline | 2.51 | 2 |
| 282 | Nc2ccc(c1ccccc1)cc2 | 4-aminobiphenyl | 4.35 | 2 |
| 283 | Cc1c(N(=O)=O)ccc(N)c1 | 3-methyl-4-nitroaniline | 1.64 | 2 |
| 284 | C(c1ccccc1)(=O)c2ccc(cc2)N | 4-benzoylaniline | 2.24 | 2 |
| 285 | [N+](=O)([O-])c1c(C)cc(cc1C)N | 3,5-dimethyl-4-nitrobenzenamine | 2.54 | 2 |
| 286 | [N+](=O)([O-])c1c(C)ccc(N)c1 | 2-nitro-p-toluidine | 0.40 | 2 |
| 287 | S(C)(=O)(=O)c1ccc(cc1)N | 4-methylsulfonylaniline | 1.35 | 2 |
| 288 | N(=O)(=O)c1c(Cl)ccc(N)c1 | 4-chloro-3-nitro-benzenamine | 1.90 | 2 |
| 289 | C(F)(F)(F)c1ccc(cc1)N | p-trifluoromethylaniline | 2.45 | 2 |
| 290 | C(OC)(=O)c1ccc(cc1)N | methyl-p-aminobenzoate | 2.47 | 2 |
| 291 | C(OCCCC)(=O)c1ccc(cc1)N | butyl-p-aminobenzoate | 2.47 | 2 |
| 292 | C(OCCC)(=O)c1ccc(cc1)N | propyl-p-aminobenzoate | 2.49 | 2 |
| 293 | C(OCC)(=O)c1ccc(cc1)N | p-aminobenzoic acid, ethyl ester | 2.51 | 2 |
| 294 | c1(Cl)c(Cl)ccc(N)c1 | 3,4-dichloroaniline | 2.97 | 2 |
| 295 | C(F)(F)(F)c1cccc(N)c1 | 3-trifluoromethylaniline | 3.49 | 2 |
| 296 | c1c(cccc1N)Br | m-bromoaniline | 3.58 | 2 |
| 297 | c1c(cccc1N)I | 3-iodo-benzenamine | 3.61 | 2 |
| 298 | c1(ccc(cc1)I)N | 4-iodo-benzenamine | 3.78 | 2 |
| 299 | c1(ccc(cc1)Br)N | p-bromoaniline | 3.86 | 2 |
| 300 | c1(C)cc(ccc1Br)N | 3-methyl-4-bromoaniline | 4.05 | 2 |

| | | | | |
|---|---|---|---|---|
| 301 | c1(ccccc1N)C(O)=O | 2-aminobenzoic acid | 2.14 | 2 |
| 302 | c1(ccccc1O)N | o-aminophenol | 4.84 | 2 |
| 303 | [N+](=O)([O-])c1ccc(c(N)c1)O | 2-amino-4-nitrophenol | 3.10 | 2 |
| 304 | c1(Br)c(N)ccc(Br)c1 | 2,4-dibromoaniline | 2.30 | 2 |
| 305 | [N+](=O)([O-])c1cc(C)ccc1N | 3-nitro-4-toluidine | 3.03 | 2 |
| 306 | c1(ccccc1N)c2ccccc2 | 2-aminobiphenyl | 3.83 | 2 |
| 307 | [N+](=O)([O-])c1cc(Cl)c(c(Cl)c1)N | 2,6-dichloro-4-nitroaniline | -2.55 | 2 |
| 308 | [N+](=O)([O-])c1cc(C)c(c(C)c1)N | 2,6-dimethyl-4-nitrobenzenamine | 0.98 | 2 |
| 309 | c1(N)c(Cl)ccc(Cl)c1 | 2,5-dichloroaniline | 2.05 | 2 |
| 310 | c1(c(N)ccc(c1)[N+](=O)[O-])[N+](=O)[O-] | 2,4-dinitroaniline | -4.25 | 2 |
| 311 | [N+](=O)([O-])c1c(N)ccc(Cl)c1 | 4-chloro-2-nitroaniline | -1.02 | 2 |
| 312 | [N+](=O)([O-])c1ccc(c(Cl)c1)N | 2-chloro-4-nitroaniline | -0.94 | 2 |
| 313 | c1(N)c(F)c(F)c(c(F)c1F)F | 2,3,4,5,6-pentafluoroaniline | -0.28 | 2 |
| 314 | c1(N)c(cccc1Cl)Cl | 2,6-dichloroaniline | 0.42 | 2 |
| 315 | N(=O)(=O)c1c(N)ccc(OC)c1 | 4-methoxy-2-nitro-benzenamine | 0.77 | 2 |
| 316 | [N+](=O)([O-])c1ccc(c(C)c1)N | 4-nitro-2-toluidine | 1.04 | 2 |
| 317 | c1(Cl)c(cccc1N)Cl | 2,3-dichloroaniline | 1.76 | 2 |
| 318 | c1(Cl)c(N)ccc(Cl)c1 | 2,4-dichloroaniline | 2.00 | 2 |
| 319 | c1(ccccc1N)C(OCC)=O | o-aminobenzoic acid, ethyl ester | 2.18 | 2 |
| 320 | c1(ccccc1N)C(OC)=O | methyl anthranilate | 2.23 | 2 |
| 321 | [N+](=O)([O-])c1ccc(c(N)c1)C | 5-nitro-2-toluidine | 2.35 | 2 |
| 322 | c1(c(C)c(C)c(c(C)c1C)N)[N+](=O)[O-] | 2,3,5,6-tetramethyl-4-nitrobenzenamine | 2.36 | 2 |
| 323 | [N+](=O)([O-])c1ccc(c(N)c1)OC | 2-methoxy-5-nitroaniline | 2.49 | 2 |
| 324 | c1(ccccc1Br)N | o-bromoaniline | 2.53 | 2 |
| 325 | c1(ccccc1I)N | 2-iodoaniline | 2.60 | 2 |
| 326 | N(=O)(=O)c1cccc(c1N)N(=O)=O | 2,6-dinitroaniline | -5.00 | 2 |
| 327 | c1(N)c(Cl)cc(cc1Cl)Cl | 2,4,6-trichloroaniline | -0.03 | 2 |
| 328 | c1c(Cl)c(Cl)cc(Cl)c1N | 2,4,5-trichloroaniline | 1.09 | 2 |
| 329 | c1(N)c(OC)ccc(OC)c1 | 2,5-dimethoxyaniline | 3.93 | 2 |

**Fluorophenols**

| | | | | |
|---|---|---|---|---|
| 330 | Oc1ccc(F)cc1F | 2,4-difluorophenol | 8.58 | 4 |
| 331 | Oc1c(F)cccc1F | 2,6-difluorophenol | 7.51 | 4 |
| 332 | Oc1c(F)c(F)cc(F)c1F | 2,3,5,6-tetrafluorophenol | 6 | 4 |

**Methoxyphenols**

| | | | | |
|---|---|---|---|---|
| 333 | COc1cc(CO)ccc1O | 4-(hydroxymethyl)-2-(methoxy)phenols | 9.78 | 5 |
| 334 | COCc1ccc(O)c(OC)c1 | 2-(methyloxy)-4-[(methyloxy)methyl]phenol | 9.79 | 5 |
| 335 | COC(=O)c1ccc(O)c(OC)c1 | methyl 4-hydroxy-3-(methyloxy)benzoate | 8.3 | 5 |
| 336 | COc1cc(CCO)ccc1O | 4-(2-hydroxyethyl)-2-(methoxy)phenol | 10.09 | 5 |
| 337 | COc1cc(ccc1O)C(C)O | 4-(1-hydroxyethyl)-2-(methoxloxy)phenol | 9.83 | 5 |
| 338 | COC(C)c1ccc(O)c(OC)c1 | 2-(methyloxy)-4-[1-(methyloxy)ethyl]phenol | 9.75 | 5 |
| 339 | COc1cc(ccc1O)C(O)CO | 1-[4-hydroxy-3-(methyloxy)phenyl]-1,2-ethanediol | 9.5 | 5 |
| 340 | COc1cc(ccc1O)C(C)=O | 1-{4-hydroxy-3-(methyloxy)phenyl]ethanone | 7.81 | 5 |
| 341 | CCCc1ccc(O)c(OC)c1 | 2-(methyloxy)-4-propylphenol | 9.85 | 5 |
| 342 | COc1cc(\C=C\CO)ccc1O | 4-[(1E)-3-hydroxy-1-propen-1-yl]-2-(methyloxy)phenol | 9.54 | 5 |
| 343 | COc1cc(\C=C\C=O)ccc1O | (2E)-3-[4-hydroxy-3-(methyloxy)phenyl]-2-propenal | 7.94 | 5 |
| 344 | CCC(O)c1ccc(O)c(OC)c1 | 4-(1-hydroxypropyl)-2-(methyloxy)phenol | 9.83 | 5 |
| 345 | CCC(=O)c1ccc(O)c(OC)c1 | 1-[4-hydroxy-3-(methyloxy)phenyl]-1-propanone | 7.98 | 5 |
| 346 | COc1cc(ccc1O)C(=O)C(C)O | 2-hydroxy-1-[4-hydroxy-3-(methyloxy)phenyl]-1-propanone | 7.32 | 5 |
| 347 | COc1cc(ccc1O)C(O)C(CO)Oc1ccccc1OC | 1-[4-hydroxy-3-(methyloxy)phenyl]-2-{[2-(methyloxy)phenl]oxy}-1,3-propanediol | 9.88 | 5 |
| 348 | COCc1cc(\C=C/Oc2ccccc2OC)ccc1O | 2-[methyloxy)methyl]-4-((Z)-2-{[2-methyloxy)phenyl]oxy}ethenyl)phenol | 9.49 | 5 |

**Meta/Para-Nitrophenols**

| | | | | |
|---|---|---|---|---|
| 349 | Oc1ccc(c(F)c1)[N+]([O-])=O | 3-fluoro-4-nitrophenol | 5.3 | 6 |
| 350 | Oc1cc(F)c(c(F)c1)[N+]([O-])=O | 3,5-difluoro-4-nitrophenol | 4.4 | 6 |
| 351 | Cc1cc(O)ccc1[N+]([O-])=O | 3-methyl-4-nitrophenol | 7.29 | 7 |
| 352 | Cc1cc(O)cc(C)c1[N+]([O-])=O | 3,5-dimetyl-4-nitrophenol | 8.25 | 8 |
| 353 | Oc1ccc(c(Cl)c1)[N+]([O-])=O | 3-chloro-4-nitrophenol | 6.49 | 8 |

**Meta-Anilines**

| | | | | |
|---|---|---|---|---|
| 354 | Nc1cccc(N)c1 | 3-aminoaniline | 4.88 | 9 |
| 355 | Nc1cccc(Cl)c1 | 3-chloroaniline | 3.34 | 9 |
| 356 | Nc1cccc(c1)C#N | 3-cyanoaniline | 2.76 | 9 |
| 357 | Nc1cccc(F)c1 | 3-fluoroaniline | 3.59 | 9 |
| 358 | COc1cccc(N)c1 | 3-methoxyaniline | 4.2 | 9 |
| 359 | Cc1cccc(N)c1 | 3-methylaniline | 4.69 | 9 |
| 360 | Nc1cccc(c1)[N+]([O-])=O | 3-nitroaniline | 2.5 | 9 |
| 361 | Cc1cc(C)cc(N)c1 | 3,4-dimethylaniline | 5.17 | 9 |
| 362 | Nc1ccc(O)c(N)c1 | 3-amino-4-hydroxyaniline | 5.7 | 9 |
| 363 | COc1ccc(N)cc1Br | 3-bromo-4-methoxyaniline | 4.08 | 9 |
| 364 | Cc1ccc(N)cc1Br | 3-bromo-4-methylaniline | 3.98 | 9 |
| 365 | Cc1ccc(N)cc1Cl | 3-chloro-4-methylaniline | 4.05 | 9 |
| 366 | Nc1cc(Br)cc(Br)c1 | 3,5-dibromoaniline | 2.34 | 9 |
| 367 | COc1cc(N)cc(OC)c1 | 3,5-dimethoxyaniline | 3.82 | 9 |
| 368 | Cc1cc(C)cc(N)c1 | 3,5-dimethylaniline | 4.91 | 9 |
| 369 | COc1cc(N)cc(Cl)c1 | 3-chloro-5-methoxyaniline | 3.1 | 9 |
| 370 | COc1cc(N)cc(c1)[N+]([O-])=O | 3-methoxy-5-nitroaniline | 2.11 | 9 |
| 371 | Nc1cc(Br)c(O)c(Br)c1 | 3,5-dibromo-4-hydroxyaniline | 3.2 | 9 |
| 372 | COc1c(Br)cc(N)cc1Br | 3,5-dibromo-4-methoxyaniline | 2.98 | 9 |
| 373 | Cc1c(Br)cc(N)cc1Br | 3,5-dibromo-4-methylaniline | 2.87 | 9 |

**Hydroxybenzoic Acids**

| | | | | |
|---|---|---|---|---|
| 373 | OC(=O)c1ccccc1O | 2-hydroxybenzoic acid | 2.98 | 10 |
| 374 | OC(=O)c1cccc(O)c1 | 3-hydroxybenzoic acid | 4.08 | 10 |
| 375 | OC(=O)c1ccc(O)cc1 | 4-hydroxybenzoic acid | 4.58 | 10 |
| 376 | OC(=O)c1cccc(O)c1O | 2,3-hydroxybenzoic acid | 2.98 | 10 |
| 377 | OC(=O)c1ccc(O)cc1O | 2,4-hydroxybenzoic acid | 3.29 | 10 |
| 378 | OC(=O)c1cc(O)ccc1O | 2,5-hydroxybenzoic acid | 2.97 | 10 |
| 379 | OC(=O)c1c(O)cccc1O | 2,6-hydroxybenzoic acid | 1.3 | 10 |

| | | | | |
|---|---|---|---|---|
| 380 | OC(=O)c1ccc(O)c(O)c1 | 3,4-hydroxybenzoic acid | 4.48 | 10 |
| 381 | OC(=O)c1cc(O)cc(O)c1 | 3,5-hydroxybenzoic acid | 4.04 | 10 |
| 382 | OC(=O)c1c(O)cc(O)cc1O | 2,4,6-hydroxybenzoic acid | 1.68 | 10 |
| 383 | OC(=O)c1cc(O)c(O)c(O)c1 | 3,4,5-hydroxybenzoic acid | 4.19 | 10 |
| 384 | OC(=O)c1ccccc1 | hydroxybenzoic acid | 4.2 | 10 |

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