Experimental Properties of Test Compounds

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ***Molecule ID*** | ***Structure*** | ***mp (°C)a*** | ***% Stability aq. buffer pH 7.4 b*** | ***Intrinsic solubility (mol/L)c*** | ***logP d*** | ***logD7.4e*** | ***PAMPA*** | | | ***pKaj*** |
| ***Pe (cm/s)g*** | ***% retentionh*** | ***logPappi*** |
| **SM25** |  | 107.8–108.5 | 100.0 | 9.97E–4 | 2.67 ±0.01 | –0.09 | 1.64E–6 | –3.05E-2 | –5.79 | 4.49 ±0.04 |
| **SM26** |  | 76.2­–78.4 | 91.4 | 8.65E–2 | 1.04 ±0.01 | –0.87 | 1.00E–06 | –5.00E–2 | –6.00 | 4.91  ±0.01 |
| **SM27** |  | ND§ | 100.0 | 8.71E–2 | ‡ | 1.56† | 6.79E–6 | –3.20E–2 | –5.17 | 10.45 ±0.01 |
| **SM28** |  | 135.3–136.8 | 94.5 | 1.62E–2 | ‡ | 1.18† | 2.11E–6 | -1.20E-2 | –5.68 | >12 |
| **SM29** |  | 71.4–71.9 | 100.0 | 2.65E–2 | 1.61 ±0.03 | 1.61 | 8.44E–6 | 0.157 | –5.1 | 10.05 ±0.01 |
| **SM30** |  | 105.8–107.2 | 94.1 | 6.38E–4 | ‡ | 2.76† | 7.06E–6 | 0.260 | –5.2 | 10.29 ±0.12 |
| **SM31** |  | ND | 93.7 | 3.47E–2 | ‡ | 1.96† | 1.02E–5 | 5.89E–2 | –4.99 | 11.02 ±0.01 |
| **SM32** |  | 115.2–116.0 | 91.5 | 1.43E–3 | ‡ | 2.44† | 1.46E–05 | 0.439 | –4.8 | 10.45 ±0.02 |
| **SM33** |  | 74.2–75.8 | 92.8 | 1.10E–3 | ‡ | 2.96† | ND | ND | ND | >12 |
| **SM34** |  | 56.6–58.9 | 93.5 | 2.20E–3 | ‡ | 2.83† | 1.14E–5 | 0.373 | –4.9 | 11.93 ±0.05 |
| **SM35** |  | 151.2–154.2 | 100.0 | 2.20E–2 | 0.88 ±0.02 | 0.87 | ND | ND | ND | 9.87 ±0.01 |
| **SM36** |  | 135.3–136.8 | 90.3 | 4.268E–2 | ‡ | 0.76† | 2.91E–6 | 5.07E–2 | –5.54 | 9.80 ±0.06 |
| **SM37** |  | 127.1–127.8 | 93.4 | 1.06E–2 | ‡ | 1.45† | 3.41E–6 | 7.13E–2 | –5.47 | 10.33 ±0.02 |
| **SM38** |  | 108.3–108.7 | 100.0 | 4.32E–2 | ‡ | 1.03† | 3.66E–06 | –3.00E-3 | –5.4 | 9.44 ±0.02 |
| **SM39** |  | 182.5–184.2 | 98.3 | 1.06E-3 | ‡ | 1.89† | ND | ND | ND | 10.22 ±0.15 |
| **SM40** |  | 100.2–101.5 | 100.0 | 8.16E–3 | 1.83 ±0.05 | 1.82 | 4.43E–6 | 0.105 | –5.35 | 9.58 ±0.01 |
| **SM41** |  | 158.0–158.8 | 97.7 | 3.85E–2 | 1.97 ±0.01 | –0.21 | 1.16E–6 | 3.42E–2 | –5.94 | 5.22 ±0.01 |
| **SM42** |  | 164.8–166.0 | 95.5 | 2.17E–3 | 1.76 ±0.03 | 0.99 | 5.79E–6 | –4.81E–2 | –5.24 | 6.62 ±0.02 |
| **SM43** |  | 152.5–152.9 | 97.3 | 2.36E–2 | 2.51 ±0.01 | 0.72 | 2.87E–6 | 0.131 | –5.54 | 5.62 ±0.02 |
| **SM44** |  | 156.0–157.5 | 93.5 | 1.05E–2 | 1.16 ±0.03 | 0.06 | 2.42E–6 | –4.07E–2 | –5.62 | 6.34 ±0.01 |
| **SM45** |  | 163.7–164.5 | 93.3 | 3.62E–4 | 2.55 ±0.04 | 1.06 | 4.09E–6 | 2.76E–4 | –5.39 | 5.93 ±0.05 |
| **SM46** |  | 158.5–159.7 | 93.9 | 2.75E–3 | 1.72 ±0.01 | 0.69 | 3.77E–6 | –4.43E–2 | –5.42 | 6.42 ±0.01 |

a Melting point of crystalline material; b Test compound (%) remaining after 5 h of incubation at rt in aqueous buffer (pH 7.4) as determined by LC/MS analyses; c Intrinsic solubility determined from the general solubility equation (GSE) by using experimentally determined logP and mp values; d Log of the partition coefficient between *n*-octanol and water (unless otherwise noted, logP determinations were conducted via potentiometric titrations using a Sirius T3, Pion); e Log of the distribution coefficient between *n*-octanol and aqueous buffer at pH 7.4 (unless otherwise noted, logD7.4 determinations were conducted via potentiometric titrations using a Sirius T3, Pion); f Calculated values using ChemAxon37; g Effective permeability (PAMPA assay run by Analiza); h Membrane retention; i Log of the apparent permeability coefficient (*Papp*); j p*K*a values determined by potentiometric titrations using a Sirius T3, Pion (values in brackets are from 30); § Test compound was an oil; † logD7.4 value determined via shake-flaskassay (experiment run by Analiza); ‡ logP value is considered equal to the logD7.4 as these compounds exhibit p*K*a values >9.4; ND = not determined.