

m-Octopamine, N-DTFMB-TMS

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| Other names: | m-Octopamine, DTFMB-TMS |
| Inchi: | InChI=1S/C23H29F6NO3Si2/c1-34(2,3)32-19-9-7-8-15(12-19)20(33-35(4,5)6)14-30-21(3 |
| InchiKey: | TXMHBEXMPLFNAE-UHFFFAOYSA-N |
| Formula: | C23H29F6NO3Si2 |
| SMILES: | C[Si](C)(C)Oc1cccc(C(CNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)O[Si](C)(C)C)c1 |
| Mol. weight [g/mol]: | 537.64 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.92 | | Crippen Method |
| logp | 7.260 | | Crippen Method |
| rinsol | 2226.00 | | NIST Webbook |
| rinsol | 2226.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R54139&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| rinsol: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/123-276-9/m-Octopamine-N-DTFMB-TMS.pdf>

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