

5-Hydroxytryptamine, DTFMB-TMS

Inchi: InChI=1S/C22H22F6N2O2Si/c1-33(2,3)32-17-4-5-19-18(11-17)13(12-30-19)6-7-29-20(3)
InchiKey: RFGQAPJCPWMQCL-UHFFFAOYSA-N
Formula: C22H22F6N2O2Si
SMILES: C[Si](C)(C)Oc1ccc2[nH]cc(CCNC(=O)c3cc(C(F)(F)F)cc(C(F)(F)F)c3)c2c1
Mol. weight [g/mol]: 488.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.09		Crippen Method
logp	5.910		Crippen Method
rinpol	2846.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R54054&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/54-306-2/5-Hydroxytryptamine-DTFMB-TMS.pdf>

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