

Dopamine, N-DTFMB-TMS

Inchi: InChI=1S/C23H29F6NO3Si2/c1-34(2,3)32-19-8-7-15(11-20(19)33-35(4,5)6)9-10-30-21(3)
InchiKey: PYXIZYRTPJQVIZ-UHFFFAOYSA-N
Formula: C23H29F6NO3Si2
SMILES: C[Si](C)(C)Oc1ccc(CCNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 537.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	7.124		Crippen Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		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=R164957&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-704-9/Dopamine-N-DTFMB-TMS.pdf>

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