

Noradrenaline, DTFMB-TBDMS

Inchi: InChI=1S/C36H57F6NO4Si3/c1-32(2,3)48(10,11)45-28(18-19-43-31(44)25-20-26(35(37,
InchiKey: JWANAIDRZKSHJX-MUUNZHRXSA-N
Formula: C36H57F6NO4Si3
SMILES: CC(C)(C)[Si](C)(C)Oc1ccc(C(CCNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)O[Si](C)(C)C(C)(C)
Mol. weight [g/mol]: 766.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.11		Crippen Method
logp	12.375		Crippen Method
rinpol	3010.00		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=R389705&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/36-372-9/Noradrenaline-DTFMB-TBDMS.pdf>

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