

Noradrenaline, N-HFB-O-TMS

Inchi: InChI=1S/C21H34F7NO4Si3/c1-34(2,3)31-15-11-10-14(12-16(15)32-35(4,5)6)17(33-36(7
InchiKey: FEABORWAPKZVDG-UHFFFAOYSA-N
Formula: C21H34F7NO4Si3
SMILES: C[Si](C)(C)Oc1ccc(C(CNC(=O)C(F)(F)C(F)(F)C(F)(F)F)O[Si](C)(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 581.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	6.956		Crippen Method
rinpol	1949.00		NIST Webbook
rinpol	1949.00		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=R139194&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/115-178-7/Noradrenaline-N-HFB-O-TMS.pdf>

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