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)(
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:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389705&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.chemeo.com/cid/36-372-9/Noradrenaline-DTFMB-TBDMS.pdf

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