

Noradrenaline, DTFMB-TMS

Other names:	Noradrenaline, N-DTFMB-TMS
Inchi:	InChI=1S/C26H37F6NO4Si3/c1-38(2,3)35-21-11-10-17(14-22(21)36-39(4,5)6)23(37-40(7
InchiKey:	RAMMWEIIFWOGPV-UHFFFAOYSA-N
Formula:	C26H37F6NO4Si3
SMILES:	C[Si](C)(C)Oc1ccc(C(CNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)O[Si](C)(C)C)cc1O[Si](C)(C
Mol. weight [g/mol]:	625.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	8.474		Crippen Method
rinpol	2391.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R315709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/114-809-7/Noradrenaline-DTFMB-TMS.pdf>

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