

N-(Trifluoroacetyl)-O,O'-bis(trimethylsilyl) dopamine

Other names:	Dopamine, N-TFA-O-TMS
Inchi:	InChI=1S/C16H26F3NO3Si2/c1-24(2,3)22-13-8-7-12(11-14(13)23-25(4,5)6)9-10-20-15(2)
InchiKey:	ZCEWWXVUIBGTRB-UHFFFAOYSA-N
Formula:	C16H26F3NO3Si2
SMILES:	C[Si](C)(C)Oc1ccc(CCNC(=O)C(F)(F)F)cc1O[Si](C)(C)C
Mol. weight [g/mol]:	393.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.75		Crippen Method
logp	4.335		Crippen Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		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=U72256&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/121-568-7/N-Trifluoroacetyl-O-O-bis-trimethylsilyl-dopamine.pdf>

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