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/ci990307l
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