Octopamine, N-TFA-O-TMS

Inchi: InChI=1S/C16H26F3NO3Si2/c1-24(2,3)22-13-9-7-12(8-10-13)14(23-25(4,5)6)11-20-15(2
InchiKey: SASUBSUPDWOBGU-UHFFFAOYSA-N
Formula: C16H26F3NO3Si2
SMILES: C[Si](C)(C)Oc1ccc(C(CNC(=O)C(F)(F)F)O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 393.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	4.471		Crippen Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R208483&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