2-{3,4-Bis[(trimethylsilyl)oxy]phenyl}ethanamine

Other names: Dopamine, bis-TMS
Inchi: InChI=1S/C14H27NO2Si2/c1-18(2,3)16-13-8-7-12(9-10-15)11-14(13)17-19(4,5)6/h7-8,11
InchiKey: MTTHITZIWQBJHX-UHFFFAOYSA-N
Formula: C14H27NO2Si2
SMILES: C[Si](C)(C)Oc1ccc(CCN)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 297.54

Physical Properties

Property code	Value	Unit	Source
log10ws	0.28		Crippen Method
logp	3.615		Crippen Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		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=U408151&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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