Octopamine, N-isoBOC, O-TBDMS

Inchi: InChI=1S/C25H47NO4Si2/c1-19(2)18-28-23(27)26-17-22(30-32(11,12)25(6,7)8)20-13-15
InchiKey: JWZDTDRIMOJIER-UHFFFAOYSA-N
Formula: C25H47NO4Si2
SMILES: CC(C)COC(=O)NCC(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 481.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	7.516		Crippen Method
rinpol	2789.00		NIST Webbook
rinpol	2789.00		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=R392791&Units=SI

Legend

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