m-Octopamine, DTFMB-TBDMS

Inchi: InChI=1S/C29H41F6NO3Si2/c1-26(2,3)40(7,8)38-23-13-11-12-19(16-23)24(39-41(9,10)2
InchiKey: OBGFFTDPWXNZAM-UHFFFAOYSA-N
Formula: C29H41F6NO3Si2
SMILES: CC(C)(C)[Si](C)(C)Oc1cccc(C(CNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)O[Si](C)(C)C(C)(C
Mol. weight [g/mol]: 621.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	9.601		Crippen Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R54125&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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