p-Octopamine, DTFMB-TBDMS

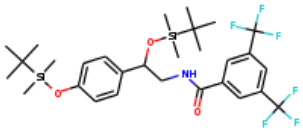
InChI: InChI=1S/C29H41F6NO3Si2/c1-26(2,3)40(7,8)38-23-13-11-19(12-14-23)24(39-41(9,10)27(4,5)6)18-36-25(37)20-15-21(28(30,31)32)17-22(16-20)29(33,34)35/h11-17,24H,18H2,1-10H3,(H,36,37)

InChI Key: GNUMIRWFEUSDSJ-UHFFFAOYSA-N

Formula: C29H41F6NO3Si2

SMILES: CC(C)(C)[Si](C)(C)Oc1ccc(C(CNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)O[Si](C)(C)C(C)(C)C)cc1

Molecular Weight: 621.80



Physical Properties

Property	Value	Unit	Source
*log*P$_{oct/wat}$	9.60		Crippen Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C29H41F6NO3Si2/c1-26(2,3)40(7,8)38-23-13-11-19(12-14-23)24(39-41(9,10)27(4,5)6)18-36-25(37)20-15-21(28(30,31)32)17-22(16-20)29(33,34)35/h11-17,24H,18H2,1-10H3,(H,36,37)

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .