

# p-Octopamine, DTFMB-TBDMS

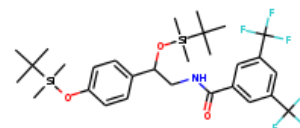
**InChI:** InChI=1S/C29H41F6NO3Si2/c1-26(2,3)40(7,8)38-23-13-11-19(12-14-23)24(39-41(9,10)27(4,5)6)18-36-25(37)20-15-21(28(30,31)32)17-22(16-20)29(33,34)35/h11-17,24H,18H2,1-10H3,(H,36,37)

**InChI Key:** GNUMIRWFEUSDSJ-UHFFFAOYSA-N

**Formula:** C<sub>29</sub>H<sub>41</sub>F<sub>6</sub>NO<sub>3</sub>Si<sub>2</sub>

**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
$\log P_{\text{oct/wat}}$	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,\(H,36,37\)](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/ci9903071>

## Legend

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

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