

# 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)2  
**InchiKey:** 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)  
**Mol. weight [g/mol]:** 621.80

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	9.601		Crippen Method
rinpol	2692.00		NIST Webbook
rinpol	2692.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R54189&Units=SI>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/67-649-8/p-Octopamine-DTFMB-TBDMS.pdf>

Generated by Cheméo on 2024-04-23 13:36:59.944820019 +0000 UTC m=+16168668.865397352.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.