

# Octopamine, N-TFA-O-TMS

**Inchi:** InChI=1S/C16H26F3NO3Si2/c1-24(2,3)22-13-9-7-12(8-10-13)14(23-25(4,5)6)11-20-15(2)  
**InchiKey:** SASUBSUPDWOBGU-UHFFFAOYSA-N  
**Formula:** C16H26F3NO3Si2  
**SMILES:** C[Si](C)(C)Oc1ccc(C(CNC(=O)C(F)(F)F)O[Si](C)(C)C)cc1  
**Mol. weight [g/mol]:** 393.55

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	4.471		Crippen Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R208483&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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<https://www.cheméo.com/cid/115-528-8/Octopamine-N-TFA-O-TMS.pdf>

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