

# Tyramine, PFB-TMS

**Inchi:** InChI=1S/C18H18F5NO2Si/c1-27(2,3)26-11-6-4-10(5-7-11)8-9-24-18(25)12-13(19)15(21)  
**InchiKey:** AQUQVACAECVICT-UHFFFAOYSA-N  
**Formula:** C18H18F5NO2Si  
**SMILES:** C[Si](C)(C)Oc1ccc(CCNC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1  
**Mol. weight [g/mol]:** 403.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	4.568		Crippen Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		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=R305801&Units=SI>

## 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.chemeo.com/cid/124-922-0/Tyramine-PFB-TMS.pdf>

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