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/ci990307l
Crippen Method: 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