p-Tyramine, DTFMB-TMS

Other names: p-Tyramine, N-DTFMB-TMS
Inchi: InChI=1S/C20H21F6NO2Si/c1-30(2,3)29-17-6-4-13(5-7-17)8-9-27-18(28)14-10-15(19(21
InchiKey: TVDFVURRXDLERZ-UHFFFAOYSA-N
Formula: C20H21F6NO2Si
SMILES: C[Si](C)(C)Oc1ccc(CCNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1
Mol. weight [g/mol]: 449.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	5.910		Crippen Method
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R54232&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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