p-Tyramine, DTFMB-TBDMS

Inchi: InChI=1S/C23H27F6NO2Si/c1-21(2,3)33(4,5)32-19-8-6-15(7-9-19)10-11-30-20(31)16-12
InchiKey: XFEUWHPUEQTYBS-UHFFFAOYSA-N
Formula: C23H27F6NO2Si
SMILES: CC(C)(C)[Si](C)(C)Oc1ccc(CCNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1
Mol. weight [g/mol]: 491.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	7.081		Crippen Method
rinpol	2367.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R54228&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