

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(20)21)22
InchiKey:	TVDFVURRXDLERZ-UHFFFAOYSA-N
Formula:	C ₂₀ H ₂₁ F ₆ NO ₂ Si
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
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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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/119-418-6/p-Tyramine-DTFMB-TMS.pdf>

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