p-Octopamine, DTFMB-TMS

Inchi: InChI=1S/C23H29F6NO3Si2/c1-34(2,3)32-19-9-7-15(8-10-19)20(33-35(4,5)6)14-30-21(3
InchiKey: HIZOWXWPEDBLRZ-UHFFFAOYSA-N
Formula: C23H29F6NO3Si2
SMILES: C[Si](C)(C)Oc1ccc(C(CNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 537.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	7.260		Crippen Method
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R54193&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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