Ethylephrine, N-TFA-O-TMS

Other names: Ethylephrine bis-O-TMS-N-TFA
Inchi: InChI=1S/C19H32F3NO4Si2/c1-9-25-16-12-14(10-11-15(16)26-28(3,4)5)17(27-29(6,7)8)
InchiKey: XRYJGVARDKICST-UHFFFAOYSA-N
Formula: C19H32F3NO4Si2
SMILES: CCOc1cc(C(CN(C)C(=O)C(F)(F)F)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 451.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Crippen Method
logp	5.212		Crippen Method
rinpol	1851.00		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=R208403&Units=SI

Legend

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