Ephedrine, N-TFA, O-TMS

Inchi: InChI=1S/C15H22F3NO2Si/c1-11(19(2)14(20)15(16,17)18)13(21-22(3,4)5)12-9-7-6-8-10
InchiKey: DUURUAMJAWIWDF-UHFFFAOYSA-N
Formula: C15H22F3NO2Si
SMILES: CC(C(O[Si](C)(C)C)c1ccccc1)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	3.988		Crippen Method
rinpol	1548.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R56919&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