Phenylephrine, N-TFA-O-TMS

Inchi: InChI=1S/C17H28F3NO3Si2/c1-21(16(22)17(18,19)20)12-15(24-26(5,6)7)13-9-8-10-14(1
InchiKey: ONSRKWRNNNIUJY-UHFFFAOYSA-N
Formula: C17H28F3NO3Si2
SMILES: CN(CC(O[Si](C)(C)C)c1cccc(O[Si](C)(C)C)c1)C(=O)C(F)(F)F
Mol. weight [g/mol]: 407.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	4.814		Crippen Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R208512&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