Metaraminol, N-TFA, bis-O-TMS

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.13		Crippen Method
logp	4.860		Crippen Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R57046&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