Isonormethanephrine, N-TFA-O-TMS

Inchi: InChI=1S/C17H28F3NO4Si2/c1-23-13-9-8-12(10-14(13)24-26(2,3)4)15(25-27(5,6)7)11-2
InchiKey: WXBNDUVLOQIRSJ-UHFFFAOYSA-N
Formula: C17H28F3NO4Si2
SMILES: COc1ccc(C(CNC(=O)C(F)(F)F)O[Si](C)(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 423.58

Physical Properties

Property code	Value	Unit	Source
logp	4.480		Crippen Method
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R139174&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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