

Normethanephrine, N-TFA-O-TMS

Inchi: InChI=1S/C17H28F3NO4Si2/c1-23-14-10-12(8-9-13(14)24-26(2,3)4)15(25-27(5,6)7)11-2
InchiKey: JFXGGTMCDOVRAF-UHFFFAOYSA-N
Formula: C17H28F3NO4Si2
SMILES: COc1cc(C(CNC(=O)C(F)(F)F)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 423.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	4.480		Crippen Method
rinpol	1888.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R139223&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/62-494-5/Normethanephrine-N-TFA-O-TMS.pdf>

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