

Epinine, N-TFA-O-TMS

Inchi: InChI=1S/C17H28F3NO3Si2/c1-21(16(22)17(18,19)20)11-10-13-8-9-14(23-25(2,3)4)15(26)27
InchiKey: SLQQLJGJUQZDSV-UHFFFAOYSA-N
Formula: C17H28F3NO3Si2
SMILES: CN(CCc1ccc(O[Si](C)(C)C)c(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	-0.55		Crippen Method
logp	4.677		Crippen Method
rinpol	1910.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R208394&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/63-719-4/Epinine-N-TFA-O-TMS.pdf>

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