

trans-3'-Hydroxycotinine, trimethylsilyl ether

Inchi: InChI=1S/C13H20N2O2Si/c1-15-11(10-6-5-7-14-9-10)8-12(13(15)16)17-18(2,3)4/h5-7,9,
InchiKey: HYTDUAPLYVHNHI-UHFFFAOYSA-N
Formula: C13H20N2O2Si
SMILES: CN1C(=O)C(O[Si](C)(C)C)CC1c1cccnc1
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.50		Crippen Method
logp	2.205		Crippen Method
rinpol	1888.60		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=U417199&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/122-102-2/trans-3-Hydroxycotinine-trimethylsilyl-ether.pdf>

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