

Ecgonine methyl ester, trimethylsilyl ether

Inchi: InChI=1S/C13H25NO3Si/c1-14-9-6-7-10(14)12(13(15)16-2)11(8-9)17-18(3,4)5/h9-12H,6
InchiKey: ZOZZIPWQUVUYGY-UHFFFAOYSA-N
Formula: C13H25NO3Si
SMILES: COC(=O)C1C(O[Si](C)(C)C)CC2CCC1N2C
Mol. weight [g/mol]: 271.43

Physical Properties

Property code	Value	Unit	Source
log10ws	0.28		Crippen Method
logp	1.862		Crippen Method
rinpol	1575.70		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417193&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/122-096-0/Ecgonine-methyl-ester-trimethylsilyl-ether.pdf>

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