

Ecgonine, trimethylsilyl ether, trimethylsilyl ester

Inchi: InChI=1S/C15H31NO3Si2/c1-16-11-8-9-12(16)14(15(17)19-21(5,6)7)13(10-11)18-20(2,3)
InchiKey: ARJVVXRHOLBHAX-UHFFFAOYSA-N
Formula: C15H31NO3Si2
SMILES: CN1C2CCC1C(C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C2
Mol. weight [g/mol]: 329.58

Physical Properties

Property code	Value	Unit	Source
log10ws	1.39		Crippen Method
logp	3.067		Crippen Method
rinpol	1647.70		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417194&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/118-794-0/Ecgonine-trimethylsilyl-ether-trimethylsilyl-ester.pdf>

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