

Tropine, (3-cyanopropyl)dimethylsilyl ether

Inchi: InChI=1S/C14H26N2OSi/c1-16-12-6-7-13(16)11-14(10-12)17-18(2,3)9-5-4-8-15/h12-14H
InchiKey: BJWGYQIPEIAEMK-UHFFFAOYSA-N
Formula: C14H26N2OSi
SMILES: CN1C2CCC1CC(O[Si](C)(C)CCCC#N)C2
Mol. weight [g/mol]: 266.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	3.137		Crippen Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375735&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/113-462-3/Tropine-3-cyanopropyl-dimethylsilyl-ether.pdf>

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