

Ornithine, TMS

Inchi: InChI=1S/C14H36N2O2Si3/c1-19(2,3)15-12-10-11-13(16-20(4,5)6)14(17)18-21(7,8)9/h1-19
InchiKey: RCRVISHDTJFLLG-UHFFFAOYSA-N
Formula: C14H36N2O2Si3
SMILES: C[Si](C)(C)NCCCC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 348.70

Physical Properties

Property code	Value	Unit	Source
log10ws	2.81		Crippen Method
logp	3.362		Crippen Method
rinpol	1825.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R638225&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/71-780-7/Ornithine-TMS.pdf>

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