

1,4-Dimethylhistidine, TMS

Inchi: InChI=1S/C14H29N3O2Si2/c1-11-13(17(2)10-15-11)9-12(16-20(3,4)5)14(18)19-21(6,7)8
InchiKey: SDXUXEDQWSUHDP-UHFFFAOYSA-N
Formula: C14H29N3O2Si2
SMILES: Cc1ncn(C)c1CC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 327.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.00		Crippen Method
logp	2.442		Crippen Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R93458&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/31-624-4/1-4-Dimethylhistidine-TMS.pdf>

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