

Carnosine, TMS

Inchi: InChI=1S/C15H30N4O3Si2/c1-23(2,3)18-8-7-14(20)19-13(9-12-10-16-11-17-12)15(21)22
InchiKey: NXLUQYPGVPBDSQ-UHFFFAOYSA-N
Formula: C15H30N4O3Si2
SMILES: C[Si](C)(C)NCCC(=O)NC(Cc1cnc[nH]1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 370.59

Physical Properties

Property code	Value	Unit	Source
log10ws	1.32		Crippen Method
logp	1.148		Crippen Method
rinpol	2543.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400758&Units=SI>

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/75-166-5/Carnosine-TMS.pdf>

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