

«beta»-Ala, N-isoBOC TBDMS

Inchi: InChI=1S/C14H29NO4Si/c1-11(2)10-18-13(17)15-9-8-12(16)19-20(6,7)14(3,4)5/h11H,8-
InchiKey: ZDWBYZGOMZNXIH-UHFFFAOYSA-N
Formula: C14H29NO4Si
SMILES: CC(C)COC(=O)NCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 303.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	3.307		Crippen Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R260327&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/121-965-6/beta-Ala-N-isoBOC-TBDMS.pdf>

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