

Isobutyrylglycine, bis-TMS

Inchi: InChI=1S/C12H27NO3Si2/c1-10(2)12(16-18(6,7)8)13-9-11(14)15-17(3,4)5/h10H,9H2,1-8H
InchiKey: RBRFVVFPMNURDE-UHFFFAOYSA-N
Formula: C12H27NO3Si2
SMILES: CC(C)C(=NCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 289.52

Physical Properties

Property code	Value	Unit	Source
log10ws	1.69		Crippen Method
logp	3.270		Crippen Method
rinpol	1430.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1442.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R147665&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/123-235-4/Isobutyrylglycine-bis-TMS.pdf>

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