

Glycine, N-(3-methyl-1-oxobutyl)-N-(trimethylsilyl)-, trimethylsilyl ester

Other names: N-(1-Oxo-3-methylbutyl)glycine, N,O-di(trimethylsilyl) deriv.
Isovalerylglycine, N,O-(di-TMS)-

Isovalerylglycine, di-TMS

N-isovalerylglycine, 2tms derivative

Inchi: InChI=1S/C13H29NO3Si2/c1-11(2)9-12(15)14(18(3,4)5)10-13(16)17-19(6,7)8/h11H,9-10

InchiKey: VESHMUUEOMEAOM-UHFFFAOYSA-N

Formula: C13H29NO3Si2

SMILES: CC(C)CC(=O)N(CC(=O)O[Si](C)(C)C)[Si](C)(C)C

Mol. weight [g/mol]: 303.55

CAS: 55520-90-6

Physical Properties

Property code	Value	Unit	Source
log10ws	1.67		Crippen Method
logp	3.074		Crippen Method
rinpol	1510.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55520906&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

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