

Glycine, N-(3-methyl-1-oxo-2-butenyl)-N-(trimethylsilyl)-, trimethylsilyl ester

Other names: «beta»-Methyl crotonyl glycine bis(trimethylsilyl)-

Inchi: InChI=1S/C13H27NO3Si2/c1-11(2)9-12(15)14(18(3,4)5)10-13(16)17-19(6,7)8/h9H,10H2

InchiKey: RJILLMNUANBLCE-UHFFFAOYSA-N

Formula: C13H27NO3Si2

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

Mol. weight [g/mol]: 301.53

CAS: 55649-86-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.57		Crippen Method
logp	2.994		Crippen Method
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55649860&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/29-172-9/Glycine-N-3-methyl-1-oxo-2-butenyl-N-trimethylsilyl-trimethylsilyl-ester.pdf>

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