

Crotonylglycine, TMS

Other names: Glycine, N-(1-oxo-2-butenyl)-N-(trimethylsilyl)-, trimethylsilyl ester
Crotonylglycine (II), TMS
Crotonylglycine (I), TMS

Inchi: InChI=1S/C12H25NO3Si2/c1-8-9-11(15-17(2,3)4)13-10-12(14)16-18(5,6)7/h8-9H,10H2,11H3

InchiKey: LYIHLKWUJQVFRE-JDZOZJMCSA-N

Formula: C12H25NO3Si2

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

Mol. weight [g/mol]: 287.50

CAS: 55557-28-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.59		Crippen Method
logp	3.191		Crippen Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1513.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55557283&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.cheméo.com/cid/49-773-0/Crotonylglycine-TMS.pdf>

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