

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

Other names: Tiglyl glycine, bis(trimethylsilyl)-
Tiglyl glycine, 2trns derivative

Inchi:	InChI=1S/C13H27NO3Si2/c1-9-11(2)13(16)14(18(3,4)5)10-12(15)17-19(6,7)8/h9H,10H2
InchiKey:	VUISAWSCGJCPQU-PKNCBQFBNSA-N
Formula:	C13H27NO3Si2
SMILES:	CC=C(C)C(=O)N(CC(=O)O[Si](C)(C)C)[Si](C)(C)C
Mol. weight [g/mol]:	301.53
CAS:	55517-45-8

Physical Properties

Property code	Value	Unit	Source
log10ws	1.57		Crippen Method
logp	2.994		Crippen Method
rinpol	1549.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1549.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517458&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/122-820-5/Glycine-N-2-methyl-1-oxo-2-butenyl-N-trimethylsilyl-trimethylsilyl-ester-E.pdf>

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