

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

Other names:

Trimethylsilyl ([[2E)-2-methyl-2-butenoyl]amino)acetate

Tiglylglycine, mono-TMS

Tiglylglycine, TMS

Tiglylglycine, TMS ester

Tyglylglycine, mono-TMS

Inchi: InChI=1S/C10H19NO3Si/c1-6-8(2)10(13)11-7-9(12)14-15(3,4)5/h6H,7H2,1-5H3,(H,11,13)

InchiKey: ACEZAZFSJHWIDP-SOFGYWHQSA-N

Formula: C10H19NO3Si

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

Mol. weight [g/mol]: 229.35

CAS: 55517-35-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.26		Crippen Method
logp	1.447		Crippen Method
rinpol	1530.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1571.90		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1549.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517356&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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