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

Other names: 3-Methylcrotonylglycine, mono-TMS
Glycine, N-(3-methyl-2-butenoyl), mono-TMS
Inchi: InChI=1S/C10H19NO3Si/c1-8(2)6-9(12)11-7-10(13)14-15(3,4)5/h6H,7H2,1-5H3,(H,11,12
InchiKey: CIBNSCXUKAEBGH-UHFFFAOYSA-N
Formula: C10H19NO3Si
SMILES: CC(C)=CC(=O)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 229.35
CAS: 54824-02-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.26		Crippen Method
logp	1.447		Crippen Method
rinpol	1564.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1564.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54824021&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices