

Glycine, N-(1-oxobutyl)-, trimethylsilyl ester

Other names:	N-Butyrylglycine, trimethylsilyl ester N-(1-Oxobutyl)glycine, monoTMS N-Butyrylglycine, TMS N-Butyrylglycine, mono-TMS N-Butyrylglycine, TMS ester BUTYRYLGLYCINE TMS Butyrylglycine, monoTMS
Inchi:	InChI=1S/C9H19NO3Si/c1-5-6-8(11)10-7-9(12)13-14(2,3)4/h5-7H2,1-4H3,(H,10,11)
InchiKey:	MHXAOBFKXNYVNB-UHFFFAOYSA-N
Formula:	C9H19NO3Si
SMILES:	CCCC(=O)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	217.34
CAS:	55493-97-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.53		Crippen Method
logp	1.281		Crippen Method
rinpol	1420.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1461.00		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=C55493975&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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