

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

Other names:	Hexanoylglycine, TMS ester N-Hexanoylglycine, TMS ester HEXANOYLGLYCINE TMS Hexanoylglycine, mono-TMS Hexanoylglycine, tms derivative
Inchi:	InChI=1S/C11H23NO3Si/c1-5-6-7-8-10(13)12-9-11(14)15-16(2,3)4/h5-9H2,1-4H3,(H,12,
InchiKey:	XROBKRJAYNGRBG-UHFFFAOYSA-N
Formula:	C11H23NO3Si
SMILES:	CCCCCC(=O)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	245.39
CAS:	55494-05-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.31		Crippen Method
logp	2.061		Crippen Method
rinpol	1610.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55494058&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

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