

Glycine, N-(2-methyl-1-oxobutyl)-, trimethylsilyl ester

Other names:	N-2-Methylbutyrylglycine, trimethylsilyl ester 2-Methylbutyrylglycine, TMS ester Glycine, N-(2-methylbutanoyl), mono-TMS 2-Methylbutyryl glycine, TMS # 1
Inchi:	InChI=1S/C10H21NO3Si/c1-6-8(2)10(13)11-7-9(12)14-15(3,4)5/h8H,6-7H2,1-5H3,(H,11,
InchiKey:	SZZJQCDMJUGIOJ-UHFFFAOYSA-N
Formula:	C10H21NO3Si
SMILES:	CCC(C)C(=O)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	231.36
CAS:	55493-99-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.36		Crippen Method
logp	1.527		Crippen Method
rinpol	1451.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1451.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55493997&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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