

N-Valerylglycine, trimethylsilyl ester

Other names:	Valerylglycine, mono-TMS
Inchi:	InChI=1S/C10H21NO3Si/c1-5-6-7-9(12)11-8-10(13)14-15(2,3)4/h5-8H2,1-4H3,(H,11,12)
InchiKey:	IFNLBQXOFXGIFR-UHFFFAOYSA-N
Formula:	C10H21NO3Si
SMILES:	CCCCC(=O)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	231.36
CAS:	71428-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.11		Crippen Method
logp	1.671		Crippen Method
rinpol	1514.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71428916&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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