

I-Val-I-leu, trimethylsilyl ester

Other names:	Trimethylsilyl I-valyl-I-leucinate L-valyl-I-leucine, tms derivative
Inchi:	InChI=1S/C14H30N2O3Si/c1-9(2)8-11(14(18)19-20(5,6)7)16-13(17)12(15)10(3)4/h9-12H
InchiKey:	FINUQILPQXLRLI-UHFFFAOYSA-N
Formula:	C14H30N2O3Si
SMILES:	CC(C)CC(NC(=O)C(N)C(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	302.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Crippen Method
logp	1.879		Crippen Method
rinpola	1783.00		NIST Webbook
rinpola	1783.00		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=U333697&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/123-965-4/I-Val-I-leu-trimethylsilyl-ester.pdf>

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