

Val-gly, trimethylsilyl ester

Other names:	Trimethylsilyl l-valylglycinate Valylglycine, tms derivative
Inchi:	InChI=1S/C10H22N2O3Si/c1-7(2)9(11)10(14)12-6-8(13)15-16(3,4)5/h7,9H,6,11H2,1-5H3
InchiKey:	XRSBJEAFGLLIPJ-UHFFFAOYSA-N
Formula:	C10H22N2O3Si
SMILES:	CC(C)C(N)C(=O)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	246.38

Physical Properties

Property code	Value	Unit	Source
log10ws	0.81		Crippen Method
logp	0.464		Crippen Method
rinpola	1654.80		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/118-745-4/Val-gly-trimethylsilyl-ester.pdf>

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