

L-Valine, trimethylsilyl ester

Other names:	Valine trimethylsilyl ester Val, mono-TMS Val, TMS ester Valine, trimethylsilyl ester, L- Val, TMS # 1 L-valine, tms derivative
Inchi:	InChI=1S/C8H19NO2Si/c1-6(2)7(9)8(10)11-12(3,4)5/h6-7H,9H2,1-5H3/t7-/m1/s1
InchiKey:	IJGIMCZHMYSSHY-SSDOTTSWSA-N
Formula:	C8H19NO2Si
SMILES:	CC(C)C(N)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	189.33
CAS:	7480-78-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.61		Crippen Method
logp	1.348		Crippen Method
rinpol	1083.20		NIST Webbook
rinpol	1105.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7480786&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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