L-Valine, N-(trimethylsilyl)-, trimethylsilyl ester

Other names:	Valine, N-(trimethylsilyl)-, trimethylsilyl ester, L- N-(Trimethylsilyl)-L-valine trimethylsilyl ester N,O-Bis-(trimethylsilyl)valine Valine, (N,O-TMS) Valine, di-TMS Val, di-TMS Val, TMS Valine, TMS L-valine, 2tms derivative
Inchi:	InChI=1S/C11H27NO2Si2/c1-9(2)10(12-15(3,4)5)11(13)14-16(6,7)8/h9-10,12H,1-8H3/t1
InchiKey:	UJMRIWMQZDBOTB-SNVBAGLBSA-N
Formula:	C11H27NO2Si2
SMILES:	CC(C)C(N[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	261.51
CAS:	7364-44-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.55		Crippen Method
logp	2.814		Crippen Method
rinpol	1225.60		NIST Webbook
rinpol	1208.40		NIST Webbook
rinpol	1225.60		NIST Webbook
rinpol	1229.37		NIST Webbook
rinpol	1234.50		NIST Webbook
rinpol	1226.70		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1208.40		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1226.70		NIST Webbook
rinpol	1234.50		NIST Webbook
rinpol	1229.37		NIST Webbook
ripol	1289.72		NIST Webbook
ripol	1289.72		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7364445&Units=SI

Legend

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