

Valine, MTH-TMS

Inchi:	InChI=1S/C10H20N2OSSi/c1-7(2)8-9(13-15(4,5)6)12(3)10(14)11-8/h7H,1-6H3,(H,11,14)
InchiKey:	IKHWODBRZLLILN-UHFFFAOYSA-N
Formula:	C10H20N2OSSi
SMILES:	CC(C)c1[nH]c(=S)n(C)c1O[Si](C)(C)C
Mol. weight [g/mol]:	244.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	2.938		Crippen Method
rinpol	1561.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R525545&Units=SI

Legend

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

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