

Alanine, 3TMS

Inchi:	InChI=1S/C12H31NO2Si3/c1-11(12(14)15-18(8,9)10)13(16(2,3)4)17(5,6)7/h11H,1-10H3
InchiKey:	JDPKWBHZDCBTPK-UHFFFAOYSA-N
Formula:	C12H31NO2Si3
SMILES:	CC(C(=O)O[Si](C)(C)C)N([Si](C)(C)C)[Si](C)(C)C
Mol. weight [g/mol]:	305.64

Physical Properties

Property code	Value	Unit	Source
log10ws	3.46		Crippen Method
logp	3.725		Crippen Method
rinpol	1361.00		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=R576895&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/16-365-9/Alanine-3TMS.pdf>

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