

Ala-«beta»-Ala, trimethylsilyl ester

Other names:	Trimethylsilyl l-alanylalaninate Alanyl-«beta»-alanine, tms derivative
Inchi:	InChI=1S/C9H20N2O3Si/c1-7(10)9(13)11-6-5-8(12)14-15(2,3)4/h7H,5-6,10H2,1-4H3,(H,
InchiKey:	VMLAKHNLMHWGIZ-UHFFFAOYSA-N
Formula:	C9H20N2O3Si
SMILES:	CC(N)C(=O)NCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	232.35

Physical Properties

Property code	Value	Unit	Source
log10ws	0.99		Crippen Method
logp	0.218		Crippen Method
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333690&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/116-544-9/Ala-beta-Ala-trimethylsilyl-ester.pdf>

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