

Ala-gly, trimethylsilyl ester

Other names:	Trimethylsilyl d-alanylglycinate Alanylglycine, tms derivative
Inchi:	InChI=1S/C8H18N2O3Si/c1-6(9)8(12)10-5-7(11)13-14(2,3)4/h6H,5,9H2,1-4H3,(H,10,12)
InchiKey:	OIKROLCDGDKWOB-UHFFFAOYSA-N
Formula:	C8H18N2O3Si
SMILES:	CC(N)C(=O)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
log10ws	1.40		Crippen Method
logp	-0.172		Crippen Method
rinpol	1515.00		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=U333701&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/39-788-5/Ala-gly-trimethylsilyl-ester.pdf>

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