

Ala-Pro, trimethylsilyl ester

Other names:	Trimethylsilyl alanylprolinate Alanylproline, tms derivative
Inchi:	InChI=1S/C11H22N2O3Si/c1-8(12)10(14)13-7-5-6-9(13)11(15)16-17(2,3)4/h8-9H,5-7,12
InchiKey:	LPTLROMVCUUXPO-UHFFFAOYSA-N
Formula:	C11H22N2O3Si
SMILES:	CC(N)C(=O)N1CCCC1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	258.39

Physical Properties

Property code	Value	Unit	Source
log10ws	0.76		Crippen Method
logp	0.703		Crippen Method
rmpol	1717.40		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/25-853-7/Ala-Pro-trimethylsilyl-ester.pdf>

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