

dl-3-Aminoisobutyric acid, trimethylsilyl ester

Other names:	Trimethylsilyl 3-amino-2-methylpropanoate 3-Aminoisobutyric acid, TMS 3-Aminoisobutyric acid, tms derivative
Inchi:	InChI=1S/C7H17NO2Si/c1-6(5-8)7(9)10-11(2,3)4/h6H,5,8H2,1-4H3
InchiKey:	CQDDCQABWZCCOO-UHFFFAOYSA-N
Formula:	C7H17NO2Si
SMILES:	CC(CN)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	175.30

Physical Properties

Property code	Value	Unit	Source
log10ws	1.14		Crippen Method
logp	0.959		Crippen Method
rinpol	1046.30		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=U332882&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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