

«beta»-Alanine, N-(trimethylsilyl)-, trimethylsilyl ester

Other names:	B-Ala, TMS, # 1
Inchi:	InChI=1S/C9H23NO2Si2/c1-13(2,3)10-8-7-9(11)12-14(4,5)6/h10H,7-8H2,1-6H3
InchiKey:	WRNXABBYSLTNAT-UHFFFAOYSA-N
Formula:	C9H23NO2Si2
SMILES:	C[Si](C)(C)NCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	233.46
CAS:	17891-86-0

Physical Properties

Property code	Value	Unit	Source
log10ws	2.26		Crippen Method
logp	2.179		Crippen Method
rinpola	1190.00		NIST Webbook
rinpola	1190.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17891860&Units=SI

Legend

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

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