

.beta.-Alanine, 3TMS

Inchi:	InChI=1S/C12H31NO2Si3/c1-16(2,3)13(17(4,5)6)11-10-12(14)15-18(7,8)9/h10-11H2,1-9
InchiKey:	MKLCEJJSOJVLNMP-UHFFFAOYSA-N
Formula:	C12H31NO2Si3
SMILES:	C[Si](C)(C)OC(=O)CCN([Si](C)(C)C)[Si](C)(C)C
Mol. weight [g/mol]:	305.64

Physical Properties

Property code	Value	Unit	Source
logp	3.726		Crippen Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R605453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/71-898-7/beta-Alanine-3TMS.pdf>

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