

BUTYRYLGLYCINE diTMS

Inchi:	InChI=1S/C12H27NO3Si2/c1-8-9-11(15-17(2,3)4)13-10-12(14)16-18(5,6)7/h8-10H2,1-7H1
InchiKey:	DOAGALDRIZUFDK-UHFFFAOYSA-N
Formula:	C12H27NO3Si2
SMILES:	CCCC(=NCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	289.52

Physical Properties

Property code	Value	Unit	Source
log10ws	1.44		Crippen Method
logp	3.415		Crippen Method
rinpol	1470.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1470.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R273264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/23-376-9/BUTYRYLGLYCINE-diTMS.pdf>

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