

Threonine, mono-ethoxycarbonylated, mono-TBDMS

Inchi:	InChI=1S/C13H27NO5Si/c1-8-18-12(17)14-10(9(2)15)11(16)19-20(6,7)13(3,4)5/h9-10,15
InchiKey:	LDROHEUCALECQM-UHFFFAOYSA-N
Formula:	C13H27NO5Si
SMILES:	CCOC(=O)NC(C(=O)O[Si](C)(C)C(C)(C)C(C)O
Mol. weight [g/mol]:	305.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.69		Crippen Method
logp	2.030		Crippen Method
rinpol	1745.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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.cheméo.com/cid/51-918-6/Threonine-mono-ethoxycarbonylated-mono-TBDMS.pdf>

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