

threonine, N(O,S)-isoBOC TBDMS

Inchi: InChI=1S/C20H39NO7Si/c1-13(2)11-25-18(23)21-16(15(5)27-19(24)26-12-14(3)4)17(22)
InchiKey: LPSJJAQUVIDIOU-OEMAIJDKSA-N
Formula: C20H39NO7Si
SMILES: CC(C)COC(=O)NC(C(=O)O[Si](C)(C)C(C)(C)C(C)C)OC(=O)OCC(C)C
Mol. weight [g/mol]: 433.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	4.483		Crippen Method
rinpol	1887.60		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R522506&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/66-416-7/threonine-N-O-S-isoBOC-TBDMS.pdf>

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