

Thr isoBOC TBDMS #1

Inchi: InChI=1S/C15H31NO5Si/c1-10(2)9-20-14(19)16-12(11(3)17)13(18)21-22(7,8)15(4,5)6/h
InchiKey: YMFNBIUENIRVLY-UHFFFAOYSA-N
Formula: C15H31NO5Si
SMILES: CC(C)COC(=O)NC(C(=O)O[Si](C)(C)C(C)(C)C(C)O
Mol. weight [g/mol]: 333.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	2.666		Crippen Method
rinpol	1887.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R68946&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

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<https://www.cheméo.com/cid/114-541-4/Thr-isoBOC-TBDMS-1.pdf>

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