

«epsilon»-Aminocaproic acid, N-isoBOC TBDMS

Inchi: InChI=1S/C17H35NO4Si/c1-14(2)13-21-16(20)18-12-10-8-9-11-15(19)22-23(6,7)17(3,4)5
InchiKey: SLXBBEQYTBODRW-UHFFFAOYSA-N
Formula: C17H35NO4Si
SMILES: CC(C)COC(=O)NCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 345.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	4.477		Crippen Method
rinpol	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R260367&Units=SI>

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/122-918-7/epsilon-Aminocaproic-acid-N-isoBOC-TBDMS.pdf>

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