

Ethionine, N-isoBOC TBDMS

Inchi: InChI=1S/C17H35NO4SSi/c1-9-23-11-10-14(18-16(20)21-12-13(2)3)15(19)22-24(7,8)17
InchiKey: UEPDTZWUKGRDLX-UHFFFAOYSA-N
Formula: C17H35NO4SSi
SMILES: CCSCCC(NC(=O)OCC(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 377.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	4.429		Crippen Method
rinpol	2194.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R260441&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/121-273-4/Ethionine-N-isoBOC-TBDMS.pdf>

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