

«beta»-Aminoisobutyric acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C12H25NO4Si/c1-9(8-13-11(15)16-5)10(14)17-18(6,7)12(2,3)4/h9H,8H2,1-7H3
InchiKey: JUYBDFYFYFDSRU-UHFFFAOYSA-N
Formula: C12H25NO4Si
SMILES: COC(=O)NCC(C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 275.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.55		Crippen Method
logp	2.527		Crippen Method
rinpol	1668.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R562762&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/59-634-3/beta-Aminoisobutyric-acid-ethoxycarbonylated-TBDMS.pdf>

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