

B-Aminoisobutyric acid, # 2

Inchi: InChI=1S/C13H33NO2Si3/c1-13(2,12(15)16-19(9,10)11)14(17(3,4)5)18(6,7)8/h1-11H3
InchiKey: XIHNNOONGSLRX-UHFFFAOYSA-N
Formula: C13H33NO2Si3
SMILES: CC(C)(C(=O)O[Si](C)(C)C)N([Si](C)(C)C)[Si](C)(C)C
Mol. weight [g/mol]: 319.66

Physical Properties

Property code	Value	Unit	Source
log10ws	3.04		Crippen Method
logp	4.115		Crippen Method
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94147&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

Latest version available from:

<https://www.cheméo.com/cid/23-410-0/B-Aminoisobutyric-acid-2.pdf>

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