

alanine, N(O,S)-isoBOC TBDMS

Other names:	Ala isoBOC TBDMS alanine, N(O,S)-isoBOC TBDMS
Inchi:	InChI=1S/C14H29NO4Si/c1-10(2)9-18-13(17)15-11(3)12(16)19-20(7,8)14(4,5)6/h10-11H
InchiKey:	XFEYVCZFKABRCV-UHFFFAOYSA-N
Formula:	C14H29NO4Si
SMILES:	CC(C)COC(=O)NC(C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	303.47

Physical Properties

Property code	Value	Unit	Source
hvap	72.85	kJ/mol	Cheméo Relay (1.0)
logp	3.306		Crippen Method
rinpol	1702.70		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1702.70		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R68786&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/115-809-6/alanine-N-O-S-isoBOC-TBDMS.pdf>

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