

L-Isoleucine, tert-butyldimethylsilyl ester

Other names:	L-isoleucine, tbdms derivative
Inchi:	InChI=1S/C12H27NO2Si/c1-8-9(2)10(13)11(14)15-16(6,7)12(3,4)5/h9-10H,8,13H2,1-7H3
InchiKey:	OXLMRXNCBQWETL-UHFFFAOYSA-N
Formula:	C12H27NO2Si
SMILES:	CCC(C)C(N)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	245.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	2.908		Crippen Method
rinpol	1395.60		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333272&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/18-211-7/l-Isoleucine-tert-butyldimethylsilyl-ester.pdf>

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