

allo-Isoleucine, ethoxycarbonylated, TBDMS

Other names:	Isoleucine, ethoxycarbonylated, TBDMS
Inchi:	InChI=1S/C15H31NO4Si/c1-9-11(3)12(16-14(18)19-10-2)13(17)20-21(7,8)15(4,5)6/h11-14
InchiKey:	YWBPHOQYHHQYMS-UHFFFAOYSA-N
Formula:	C15H31NO4Si
SMILES:	CCOC(=O)NC(C(=O)O[Si](C)(C)C(C)(C)C(C)CC
Mol. weight [g/mol]:	317.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	3.696		Crippen Method
rinpola	1743.00		NIST Webbook
rinpola	1732.00		NIST Webbook
rinpola	1743.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R563923&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/39-813-6/allo-Isoleucine-ethoxycarbonylated-TBDMS.pdf>

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