

Ile isoBOC TBDMS

Other names:	Ile, N-isoBOC TBDMS
Inchi:	InChI=1S/C17H35NO4Si/c1-10-13(4)14(18-16(20)21-11-12(2)3)15(19)22-23(8,9)17(5,6)
InchiKey:	RZVXLGVTQIGIKL-ZIAGYGMSSA-N
Formula:	C17H35NO4Si
SMILES:	CCC(C)C(NC(=O)OCC(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	345.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	4.332		Crippen Method
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R68861&Units=SI

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/66-484-2/Ile-isoBOC-TBDMS.pdf>

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