

His isoBOC TBDMS

Other names:	His, N-isoBOC TBDMS
Inchi:	InChI=1S/C22H39N3O6Si/c1-15(2)12-29-20(27)24-18(19(26)31-32(8,9)22(5,6)7)10-17-1
InchiKey:	MEKKZOVDFSMITK-UHFFFAOYSA-N
Formula:	C22H39N3O6Si
SMILES:	CC(C)COC(=O)NC(Cc1cn(C(=O)OCC(C)C)cn1)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	469.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	4.365		Crippen Method
rinpol	2775.00		NIST Webbook
rinpol	2773.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R68857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/11-511-1/His-isoBOC-TBDMS.pdf>

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