

cis-5-hydroxypipicolinic acid, N(O,S)-isoBOC TBDMS

Inchi:	InChI=1S/C22H41NO7Si/c1-15(2)13-27-20(25)23-12-17(29-21(26)28-14-16(3)4)10-11-18
InchiKey:	OXONXQHBFUTZAY-QZTJIDSGSA-N
Formula:	C22H41NO7Si
SMILES:	CC(C)COC(=O)OC1CCC(C(=O)O[Si](C)(C)C(C)(C)C)N(C(=O)OCC(C)C)C1
Mol. weight [g/mol]:	459.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	4.970		Crippen Method
rinpol	2149.10		NIST Webbook
rinpol	2149.10		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522457&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/61-976-1/cis-5-hydroxypipicolinic-acid-N-O-S-isoBOC-TBDMS.pdf>

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