trans-5-hydroxypipecolic 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-ZWKOTPCHSA-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	2171.90		NIST Webbook
rinpol	2171.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R522511&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices