

3-hydroxy-4-methylglutamic acid, N(O,S)-isoBOC TBDMS, diastereoisomer 2

Inchi: InChI=1S/C27H53NO9Si2/c1-17(2)16-33-24(31)28-20(23(30)37-39(14,15)27(9,10)11)21
InchiKey: NDAVCWSPQMWEST-NYLDSWQDSA-N
Formula: C27H53NO9Si2
SMILES: CC(C)COC(=O)NC(C(=O)O[Si](C)(C)C(C)(C)C)C(OC(=O)OC(C)C)C(C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 591.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	6.400		Crippen Method
rinpol	2514.30		NIST Webbook
rinpol	2514.30		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R522422&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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