3,6-dideoxy-arabino-hexonic acid, 1,4-lactone, TMS

Inchi: InChI=1S/C12H26O4Si2/c1-9(15-17(2,3)4)10-8-11(12(13)14-10)16-18(5,6)7/h9-11H,8H2

InchiKey: SMFMESPJTFCMTH-UHFFFAOYSA-N

Formula: C12H26O4Si2

SMILES: CC(O[Si](C)(C)C)C1CC(O[Si](C)(C)C)C(=O)O1

Mol. weight [g/mol]: 290.50

Physical Properties

Property code	Value	Unit	Source
log10ws	1.79		Crippen Method
logp	2.762		Crippen Method
rinpol	1519.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R101134&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

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https://www.chemeo.com/cid/59-906-1/3-6-dideoxy-arabino-hexonic-acid-1-4-lactone-TMS.pdf

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