1,4-Anhydro-3-deoxypentitol-2-carboxylic acid, TMS

Inchi: InChI=1S/C12H26O4Si2/c1-17(2,3)15-9-11-7-10(8-14-11)12(13)16-18(4,5)6/h10-11H,7-9

InchiKey: IEVXRVGHUBGOBQ-UHFFFAOYSA-N

Formula: C12H26O4Si2

SMILES: C[Si](C)(C)OCC1CC(C(=O)O[Si](C)(C)C)CO1

Mol. weight [g/mol]: 290.50

Physical Properties

Property code	Value	Unit	Source
log10ws	2.25		Crippen Method
logp	2.621		Crippen Method
rinpol	1652.00		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=R100686&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices