3-Deoxy-2-C-hydroxymethyl-erythro-pentonic acid, 1,4-lactone, TMS

Inchi: InChI=1S/C15H34O5Si3/c1-21(2,3)17-11-13-10-15(14(16)19-13,20-23(7,8)9)12-18-22(4,

InchiKey: LTOICSKFAJUJMB-CFMCSPIPSA-N

Formula: C15H34O5Si3

SMILES: C[Si](C)(C)OCC1CC(CO[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O1

Mol. weight [g/mol]: 378.68

Physical Properties

Property code	Value	Unit	Source
log10ws	3.50		Crippen Method
logp	3.595		Crippen Method
rinpol	1702.00		NIST Webbook
rinpol	1702.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R487691&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