3-Deoxy-2C-(hydroxymethyl)threo-pentonic acid lactone, TMS

Inchi: InChI=1S/C17H36O5Si2/c1-16(2,3)22-17(10-11-19-23(4,5)6)12-14(21-15(17)18)13-20-24

InchiKey: VXRFBXFUZNGKOI-PBHICJAKSA-N

Formula: C17H36O5Si2

SMILES: CC(C)(C)OC1(CCO[Si](C)(C)C)CC(CO[Si](C)(C)C)OC1=O

Mol. weight [g/mol]: 376.64

Physical Properties

Property code	Value	Unit	Source
log10ws	0.60		Crippen Method
logp	3.949		Crippen Method
rinpol	1718.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R391392&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices