1,4:3,6-Dianhydromannitol, TMS

Inchi: InChI=1S/C12H26O4Si2/c1-17(2,3)15-9-7-13-12-10(8-14-11(9)12)16-18(4,5)6/h9-12H,7-
InchiKey: LJFXZWTUMDMOLO-NNYUYHANSA-N
Formula: C12H26O4Si2
SMILES: C[Si](C)(C)OC1COC2C(O[Si](C)(C)C)COC12
Mol. weight [g/mol]: 290.50

Physical Properties

Property code	Value	Unit	Source
log10ws	2.47		Crippen Method
logp	2.224		Crippen Method
rinpol	1537.00		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=R74131&Units=SI

Legend

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