2,5-Anhydromannitol, furanose, TMS

Inchi: InChI=1S/C18H44O5Si4/c1-24(2,3)19-13-15-17(22-26(7,8)9)18(23-27(10,11)12)16(21-15
InchiKey: YZGMJBIESLNGPO-XSLAGTTESA-N
Formula: C18H44O5Si4
SMILES: C[Si](C)(C)OCC1OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 452.88

Physical Properties

Property code	Value	Unit	Source
log10ws	4.66		Crippen Method
logp	4.897		Crippen Method
rinpol	1754.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R441115&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