2-deoxyglucitol, TMS

Inchi: InChI=1S/C21H54O5Si5/c1-27(2,3)22-17-16-19(24-29(7,8)9)21(26-31(13,14)15)20(25-30

InchiKey: ULCPMKYKEVLMSQ-UHFFFAOYSA-N

Formula: C21H54O5Si5

SMILES: C[Si](C)(C)OCCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 527.08

Physical Properties

Property code	Value	Unit	Source
log10ws	5.36		Crippen Method
logp	6.740		Crippen Method
rinpol	1859.70		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R488832&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