2-Deoxy-3-C-(hydroxymethyl)tetraric acid, TMS

Inchi: InChI=1S/C17H40O6Si4/c1-24(2,3)20-14-17(23-27(10,11)12,16(19)22-26(7,8)9)13-15(18

InchiKey: CUGMQWBISPXASF-QGZVFWFLSA-N

Formula: C17H40O6Si4

SMILES: C[Si](C)(C)OCC(CC(=O)O[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 452.84

Physical Properties

Property code	Value	Unit	Source
log10ws	4.85		Crippen Method
logp	4.574		Crippen Method
rinpol	1714.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R100899&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