2-Deoxy-3-C-methyltetraric acid, TMS

Inchi: InChI=1S/C14H32O5Si3/c1-14(19-22(8,9)10,13(16)18-21(5,6)7)11-12(15)17-20(2,3)4/h1
InchiKey: PQUDIQABDWAPQW-AWEZNQCLSA-N
Formula: C14H32O5Si3
SMILES: CC(CC(=O)O[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 364.66

Physical Properties

Property code	Value	Unit	Source
log10ws	3.24		Crippen Method
logp	3.743		Crippen Method
rinpol	1488.00		NIST Webbook
rinpol	1488.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R100908&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