3-Deoxy-threo-pentaric acid, TMS

Inchi: InChI=1S/C17H40O6Si4/c1-24(2,3)20-14(16(18)22-26(7,8)9)13-15(21-25(4,5)6)17(19)23
InchiKey: KJJOKCNZSWRSBI-GASCZTMLSA-N
Formula: C17H40O6Si4
SMILES: C[Si](C)(C)OC(=O)C(CC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 452.84

Physical Properties

Property code	Value	Unit	Source
log10ws	4.73		Crippen Method
logp	4.573		Crippen Method
rinpol	1733.00		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=R101367&Units=SI

Legend

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