3-Deoxy-2-C-hydroxymethyl-threo-pentaric acid, TMS

Inchi: InChI=1S/C21H50O7Si5/c1-29(2,3)24-17-21(28-33(13,14)15,20(23)27-32(10,11)12)16-1

InchiKey: WNEDAUVACAQDIF-ZYZRXSCRSA-N

Formula: C21H50O7Si5

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

Mol. weight [g/mol]: 555.04

Physical Properties

Property code	Value	Unit	Source
log10ws	5.92		Crippen Method
logp	5.795		Crippen Method
rinpol	1940.00		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=R101203&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:
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