3-Deoxy-2-C-hydroxymethyl-threo-pentonic acid, pentakis-TMS

Inchi: InChI=1S/C21H52O6Si5/c1-28(2,3)23-17-19(25-30(7,8)9)16-21(27-32(13,14)15,18-24-29

InchiKey: COPXMBFDIHFMGG-QWAKEFERSA-N

Formula: C21H52O6Si5

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

Mol. weight [g/mol]: 541.06

Physical Properties

Property code	Value	Unit	Source
log10ws	5.70		Crippen Method
logp	6.268		Crippen Method
rinpol	1919.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R101223&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