4-Deoxytetronic acid, threo-, tri-TMS

Other names: threono-4-Deoxytetronic acid, tris-TMS
Inchi: InChI=1S/C13H32O4Si3/c1-11(15-18(2,3)4)12(16-19(5,6)7)13(14)17-20(8,9)10/h11-12H
InchiKey: UFQZVEYAONLNKN-NWDGAFQWSA-N
Formula: C13H32O4Si3
SMILES: CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 336.65

Physical Properties

Property code	Value	Unit	Source
log10ws	3.32		Crippen Method
logp	3.825		Crippen Method
rinpol	1376.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1369.00		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=R51660&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.