Dihydroxyfumaric acid, TBDMS

Inchi: InChI=1S/C29H62O6Si4/c1-25(2,3)29(13,14)36-32-23(30)21(33-37(15,16)26(4,5)6)22(34

InchiKey: GOZQZHAFNXLOAY-QURGRASLSA-N

Formula: C29H62O6Si4

SMILES: CC(C)(C)C(C)(C)[SiH2]OC(=O)C(O[Si](C)(C)C(C)(C)C)=C(O[Si](C)(C)C(C)(C)C)C(=O)O

Mol. weight [g/mol]: 619.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.23		Crippen Method
logp	8.662		Crippen Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R564179&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