3-O-Methylgularic acid, TMS

Inchi: InChI=1S/C22H52O8Si5/c1-25-17(19(27-32(5,6)7)21(23)29-34(11,12)13)18(26-31(2,3)4)
InchiKey: BIWFCGHEFHVCHR-UHFFFAOYSA-N
Formula: C22H52O8Si5
SMILES: COC(C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(

Physical Properties

Property code	Value	Unit	Source
log10ws	6.19		Crippen Method
logp	5.418		Crippen Method
rinpol	1988.00		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=R101441&Units=SI

Legend

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