3-O-Methylgulonic acid, pentakis-TMS

Inchi: InChI=1S/C22H54O7Si5/c1-24-20(21(28-33(11,12)13)22(23)29-34(14,15)16)19(27-32(8,

InchiKey: GABHOMJIRKCOOC-UHFFFAOYSA-N

Formula: C22H54O7Si5

SMILES: COC(C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 571.09

Physical Properties

Property code	Value	Unit	Source
log10ws	5.97		Crippen Method
logp	5.891		Crippen Method
rinpol	1938.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R101456&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