

# 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)(C)C  
**Mol. weight [g/mol]:** 585.07

## 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/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

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