

# 3«beta»-Hydroxy-7«alpha»-methoxycholanolic acid, methyl ester, TMS

**Inchi:** InChI=1S/C29H52O4Si/c1-19(9-12-26(30)32-5)22-10-11-23-27-24(14-16-29(22,23)3)28(30)29  
**InchiKey:** JBDNEAGIZQUFGR-ZOSOAMDQSA-N  
**Formula:** C29H52O4Si  
**SMILES:** COC(=O)CCC(C)C1CCC2C3C(OC)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C  
**Mol. weight [g/mol]:** 492.81

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	7.080		Crippen Method
rinpol	3251.00		NIST Webbook
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## Sources

**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=R535309&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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