

# Methyl 23-hydroxycholelate tetrakis(trimethylsilyl)-

**Other names:** 1«beta»,3«alpha»,7«alpha»,12«alpha»-Tetrahydroxy-5«beta»-cholanic acid, methyl ester, TMS  
**Inchi:** InChI=1S/C37H74O6Si4/c1-25(17-20-34(38)39-4)28-18-19-29-35-30(24-33(37(28,29)3)4  
**InchiKey:** NSPWFCYVNJGODS-YGVKRZELSA-N  
**Formula:** C37H74O6Si4  
**SMILES:** COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C4  
**Mol. weight [g/mol]:** 727.32  
**CAS:** 111945-03-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3325.00		NIST Webbook
rinpol	3325.00		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=C111945030&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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