

# 3«alpha»,7«beta»,17«alpha»-trihydroxy-5«beta»-cholanic acid, TMS

InChI: InChI=1S/C36H72O5Si4/c1-26(16-17-32(37)40-44(10,11)12)36(41-45(13,14)15)23-20-30  
InChIKey: CQOCBDHGMLOCMN-DIMYLECUSA-N  
Formula: C36H72O5Si4  
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)C  
Mol. weight [g/mol]: 697.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	10.464		Crippen Method
rinpol	3418.00		NIST Webbook
rinpol	3419.00		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=R279955&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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