

# allo-Cholanic acid, 3«alpha»-hydroxy, Me-TMS

**Other names:** 3«alpha»-Hydroxy-5«alpha»-cholanic acid, methyl ester, TMS  
**Inchi:** InChI=1S/C28H50O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6)  
**InchiKey:** MMCLGKIAEUXBCF-IYRMHFKPSA-N  
**Formula:** C28H50O3Si  
**SMILES:** COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C  
**Mol. weight [g/mol]:** 462.78

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	7.455		Crippen Method
rinpola	3141.00		NIST Webbook
rinpola	3141.00		NIST Webbook
rinpola	3141.00		NIST Webbook
ripola	3667.00		NIST Webbook
ripola	3667.00		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=R533516&Units=SI>

## Legend

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

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