

# Cholanic acid, 12«beta»-hydroxy, Me-DMES

**Inchi:** InChI=1S/C29H52O3Si/c1-8-33(6,7)32-26-19-25-22(14-13-21-11-9-10-18-28(21,25)3)24  
**InchiKey:** DBDZGEARTPZCLG-UYKHAKLESA-N  
**Formula:** C29H52O3Si  
**SMILES:** CC[Si](C)(C)OC1CC2C(CCC3CCCCC32C)C2CCC(C(C)CCC(=O)OC)C12C  
**Mol. weight [g/mol]:** 476.81

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	7.845		Crippen Method
rinpol	3098.00		NIST Webbook
ripol	3535.00		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=R533843&Units=SI>

## Legend

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

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