

# allo-Cholanic acid, 3«beta»,7«beta»-dihydroxy, Me-DMES

**Inchi:** InChI=1S/C33H62O4Si2/c1-11-38(7,8)36-25-17-19-32(4)24(21-25)22-29(37-39(9,10)12-13)35-33-34-30-31-32  
**InchiKey:** HBVFSTTUJXVCFB-HTXRTVHSSA-N  
**Formula:** C33H62O4Si2  
**SMILES:** CC[Si](C)(C)OC1CCC2(C)C(C1)CC(O[Si](C)(C)CC)C1C2CCC2(C)C(C(C)CCC(=O)OC)C  
**Mol. weight [g/mol]:** 579.01

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	9.065		Crippen Method
rinpol	3581.00		NIST Webbook
rinpol	3581.00		NIST Webbook
ripol	4049.00		NIST Webbook
ripol	4049.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R533665&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## 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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