

# allo-Cholanic acid, 3«beta»,12«beta»-dihydroxy, Me-DMES

**Inchi:** InChI=1S/C33H62O4Si2/c1-11-38(7,8)36-25-19-20-32(4)24(21-25)14-15-26-28-17-16-27  
**InchiKey:** LNGHMHTXKIMWLA-XWPXSEOFSA-N  
**Formula:** C33H62O4Si2  
**SMILES:** CC[Si](C)(C)OC1CCC2(C)C(CCC3C2CC(O[Si](C)(C)CC)C2(C)C(C(C)CCC(=O)OC)CCO  
**Mol. weight [g/mol]:** 579.01

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	9.065		Crippen Method
rinpol	3526.00		NIST Webbook
rinpol	3526.00		NIST Webbook
ripol	3900.00		NIST Webbook
ripol	3900.00		NIST Webbook

## Sources

**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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R533541&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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