

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

**Inchi:** InChI=1S/C29H52O3Si/c1-8-33(6,7)32-22-15-17-28(3)21(19-22)10-11-23-25-13-12-24(2)  
**InchiKey:** AFFGQJQTRAVONU-OKDOANCBSA-N  
**Formula:** C29H52O3Si  
**SMILES:** CC[Si](C)(C)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCC(=O)OC)CCC32)C1  
**Mol. weight [g/mol]:** 476.81

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -5.72   |      | Crippen Method |
| logp          | 7.845   |      | Crippen Method |
| rinpol        | 3266.00 |      | NIST Webbook   |
| ripol         | 3758.00 |      | NIST Webbook   |

## Sources

**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=R533501&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

## 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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