

# Cholanic acid, 3«alpha»,6«alpha»-dihydroxy, Me-TMS

**Inchi:** InChI=1S/C31H58O4Si2/c1-21(11-14-29(32)33-4)24-12-13-25-23-20-28(35-37(8,9)10)27  
**InchiKey:** FYDBJLGZNQLQEL-HRBZGSFOSA-N  
**Formula:** C31H58O4Si2  
**SMILES:** COC(=O)CCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C  
**Mol. weight [g/mol]:** 550.96

## Physical Properties

| Property code | Value   | Unit | Source             |
|---------------|---------|------|--------------------|
| log10ws       | -6.52   |      | Cheméo Relay (1.0) |
| logp          | 8.285   |      | Crippen Method     |
| rinpol        | 3238.00 |      | NIST Webbook       |
| ripol         | 3674.00 |      | NIST Webbook       |
| tf            | 389.62  | K    | Cheméo Relay (1.0) |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**Cheméo Relay (1.0):**  
**Cheméo Relay (1.0, beta):**  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R533932&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  
**tf:** Normal melting (fusion) point

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