

# 3-«alpha»-12-«alpha»-Dihydroxy-7-keto-5-«beta»-cholanoic acid, MeTMS

InChI: InChI=1S/C31H56O5Si2/c1-20(11-14-28(33)34-4)23-12-13-24-29-25(19-27(31(23,24)3)32)/s1  
InChIKey: KBOUNKSJJJDJEM-AWKYZDGLSA-N  
Formula: C31H56O5Si2  
SMILES: COC(=O)CCC(C)C1CCC2C3C(=O)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C  
Mol. weight [g/mol]: 564.94

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	7.464		Crippen Method
rinpol	3365.00		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=R393145&Units=SI>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/45-913-8/3-alpha-12-alpha-Dihydroxy-7-keto-5-beta-cholanoic-acid-MeTMS.pdf>

Generated by Cheméo on 2024-04-23 06:10:30.654041851 +0000 UTC m=+16141879.574619163.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.