

# 3«alpha»,7«alpha»,12«alpha»-Trihydroxy-5«beta»

Other names: Homocholic acid, trimethylsilyl ether-methyl ester

**acid, MeTMS**  
InChI: InChI=1S/C35H68O5Si3/c1-24(15-14-16-32(36)37-4)27-17-18-28-33-29(23-31(35(27,28)

InchiKey: ATLPMJCJNAJKBU-WEFHNKALSA-N

Formula: C35H68O5Si3

SMILES: COC(=O)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1

Mol. weight [g/mol]: 653.17

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	9.505		Crippen Method
rinpol	3350.00		NIST Webbook
rinpol	3384.00		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=R182544&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.cheméo.com/cid/47-877-7/3-alpha-7-alpha-12-alpha-Trihydroxy-5-beta-homocholanoic-acid-MeTMS.pdf>

Generated by Cheméo on 2024-04-17 03:41:48.589549073 +0000 UTC m=+15614557.510126385.

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