

# allo-Cholanic acid, 3«alpha»,7«alpha»,12«beta»-trihydroxy,

**Me-DMES**

InChI: InChI=1S/C37H72O5Si3/c1-14-43(8,9)40-28-21-22-36(5)27(23-28)24-32(41-44(10,11)15

InChIKey: QIHGNFRQNAWOFU-DGBCUHOUSA-N

Formula: C37H72O5Si3

SMILES: CC[Si](C)(C)OC1CCC2(C)C(C1)CC(O[Si](C)(C)CC)C1C2CC(O[Si](C)(C)CC)C2(C)C(C(C

Mol. weight [g/mol]: 681.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	10.285		Crippen Method
rinsol	3512.00		NIST Webbook
ripol	3718.00		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=R533407&Units=SI>

## Legend

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

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