

# 3«alpha»,5«beta»,12«alpha»-trihydroxy-5«beta»-cholanic acid, DMESI

InChI: InChI=1S/C40H80O5Si4/c1-16-46(8,9)42-31-24-26-38(6)35-28-36(43-47(10,11)17-2)39(20,21)40  
InChIKey: DLKOXLYAEWVHNI-KCMBWTAQSA-N

Formula: C40H80O5Si4  
SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3CCC4(O[Si](C)(C)CC)CC(O[Si](C)(C)CC)CCC4  
Mol. weight [g/mol]: 753.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	12.024		Crippen Method
rinpol	3551.00		NIST Webbook
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## 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=R279742&Units=SI>  
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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