

# 3«alpha»,7«beta»,14«alpha»-trihydroxy-5«beta»-cholanic acid, TMS

InChI: InChI=1S/C36H72O5Si4/c1-26(16-17-32(37)40-44(10,11)12)29-20-23-36(41-45(13,14)15)  
InChIKey: FXIHTYHJAIHHNY-TVIBPRCASA-N  
Formula: C36H72O5Si4  
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2(O[Si](C)(C)C)C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)C  
Mol. weight [g/mol]: 697.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	10.464		Crippen Method
rinpol	3184.00		NIST Webbook
rinpol	3188.00		NIST Webbook

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279935&Units=SI>  
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)

## Legend

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

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