

# 3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-acid, DMESI

InChI: nChI=1S/C40H80O5Si4/c1-16-46(8,9)42-31-24-25-39(6)30(26-31)27-35(43-47(10,11)17  
InChIKey: KAOHKQKCNVTQEV-JTEIHBASA-N

Formula: C40H80O5Si4  
SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)CC)CC4CC(O[Si](C)(C)CC)CCC4  
Mol. weight [g/mol]: 753.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	11.880		Crippen Method
rinpol	3526.00		NIST Webbook
rinpol	3526.00		NIST Webbook

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279866&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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