

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

InChI: InChI=1S/C36H72O5Si4/c1-26(16-19-33(37)40-44(10,11)12)29-17-18-30-28-21-23-36(4)
InChIKey: VWAGPOHFACUIQM-MUZUQNTPSA-N
Formula: C36H72O5Si4
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3CCC4(O[Si](C)(C)C)CC(O[Si](C)(C)C)CCC4(C)C3
Mol. weight [g/mol]: 697.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	10.464		Crippen Method
rinpol	3322.00		NIST Webbook
rinpol	3358.00		NIST Webbook
rinpol	3322.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279757&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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.chemeo.com/cid/35-413-4/3-alpha-5-beta-12-alpha-trihydroxy-5-beta-cholan-24-oic-acid-TMS.pdf>

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