

3«alpha»,6«beta»,7«alpha»,12«beta»-Tetrahydroxy-5«beta»-cholanoic acid, MeTMS

Other names: 3«alpha»,6«beta»,7«alpha»,12«beta»-Tetrahydroxy-5«beta»-cholanoic acid, ethyl ester-trimethylsilyl ether
Inchi: InChI=1S/C37H74O6Si4/c1-25(17-20-32(38)39-4)27-18-19-28-33-29(24-31(37(27,28)3)4)
InchiKey: CAHBNWKLPVHQBG-RJXXTHDZSA-N
Formula: C37H74O6Si4
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4
Mol. weight [g/mol]: 727.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3243.00		NIST Webbook
rinpol	3243.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R271406&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: 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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