

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

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)5-6-7-8-9-10-11-12-13-14-15-16-34-35-36-37/s1-25(17-20-32(38)39-4)27-18-19-28-33-29(24-31(37(27,28)3)4)5-6-7-8-9-10-11-12-13-14-15-16-34-35-36-37/t17-20-32(38)39-4/27-18-19-28-33-29(24-31(37(27,28)3)4)5-6-7-8-9-10-11-12-13-14-15-16-34-35-36-37/m1
InchiKey: CAHBNWKLPVHQBG-OUNUWFJUSA-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	3226.00		NIST Webbook
rinpol	3226.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393254&Units=SI>

Legend

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

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