

1-«beta»,3-«alpha»,12-«alpha»-Trihydroxy-5-«beta»-cholanoic acid, MeTMS

Other names: 1-«beta»-Cholanoic acid, 1-«beta»-3-«alpha»,12-«alpha»-trihydroxy, methyl ester,
InChI: InChI=1S/C34H66O5Si3/c1-23(14-19-32(35)36-4)27-17-18-28-26-16-15-24-20-25(37-40)31-34
InchiKey: XULBSWSPHURKBG-DYXBISBCSA-N
Formula: C34H66O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C4(C)C3CC(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3296.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393096&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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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