

3-«alpha»,4-«xi»,7-«beta»-Trihydroxy-5-«beta»-cholic acid, methyl ester, TMS

InChI: InChI=1S/C34H66O5Si3B1-23(14-17-30(35)36-4)24-15-16-25-31-26(18-20-33(24,25)2)3
InChIKey: XLJGJNLLTFGJMTL-YMVPXISQSA-N

Formula: C34H66O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3464.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393001&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/15-122-9/3-alpha-4-xi-7-beta-Trihydroxy-5-beta-cholic-acid-methyl-ester-TMS.pdf>

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