

5-cholenoate, 3«beta»-hydroxy, methyl ester-trimethylsilyl ether

Inchi: InChI=1S/C28H48O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6)7)25-27-28
InchiKey: XCHAAEKPDWQLIP-NMUHBOGFSA-N
Formula: C28H48O3Si
SMILES: COC(=O)CCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 460.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	7.375		Crippen Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R493933&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/46-954-2/5-cholenoate-3-beta-hydroxy-methyl-ester-trimethylsilyl-ether.pdf>

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