

3-oxy-7«alpha»,12«alpha»-dihydroxy-5«beta»-cholesterol methyl ester-trimethylsilyl ether

Inchi: InChI=1S/C37H70O5Si3/c1-15(16-15-17-26(2)35(38)39-5)29-18-19-30-34-31(24-33(37(2)36-33)25-31)32-31
InchiKey: VIVBCUNEPIJING-ZUBOPLHASA-N

Formula: C37H70O5Si3
SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C=C(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 679.21

Physical Properties

Property code	Value	Unit	Source
logp	10.266		Crippen Method
rinpol	3545.00		NIST Webbook
rinpol	3545.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R493864&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:
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