

7«alpha»,12«alpha»-dihydroxy-3-oxy-4-chol-24-oate-O-methyloxime (1)

Other names: 7«alpha»,12«alpha»-dihydroxy-3-oxy-4-chol-24-oate, O-methyloxime (1), TMS
Inchi: InChI=1S/C34H63NO5Si3/c1-23(14-17-31(36)40-43(11,12)13)26-15-16-27-32-28(22-30)
InchiKey: GOURTNFZHFAQOS-ZECCVNMMSA-N
Formula: C34H63NO5Si3
SMILES: CON=C1C=C2CC(O[Si](C)(C)C)C3C(CC(O[Si](C)(C)C)C4(C)C(C(C)CCC(=O)O[Si](C)(C)C)
Mol. weight [g/mol]: 650.12

Physical Properties

Property code	Value	Unit	Source
logp	9.022		Crippen Method
rinpol	3285.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R492549&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/70-289-4/7-alpha-12-alpha-dihydroxy-3-oxy-4-chol-24-oate-O-methyloxime-1.pdf>

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