

Methyl 5-«beta»-cholan-3,7-dione-24-oate, oxime, TMS # 2

Inchi: InChI=1S/C31H56N2O4Si2/c1-21(11-14-28(34)35-4)24-12-13-25-29-26(16-18-31(24,25)
InchiKey: WOTVCHNATMCTKG-MPTDWEDHSA-N
Formula: C31H56N2O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3C(=NO[Si](C)(C)C)CC4CC(=NO[Si](C)(C)C)CCC4(C)C3CC
Mol. weight [g/mol]: 576.96

Physical Properties

Property code	Value	Unit	Source
logp	8.259		Crippen Method
rinpol	3392.00		NIST Webbook
rinpol	3392.00		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=R215862&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:

<https://www.chemeo.com/cid/123-128-3/Methyl-5-beta-cholan-3-7-dione-24-oate-oxime-TMS-2.pdf>

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