

Methyl 5-«beta»-cholan-3,12-dione-24-oate, oxime, TMS

Inchi: InChI=1S/C31H56N2O4Si2/c1-21(11-16-29(34)35-4)25-14-15-26-24-13-12-22-19-23(32-33)/h1-10,12-15,17-20,22-23,25-26,28-29,31-32,34-35/t16,24,30
InchiKey: VRCDGKRYZBFSLU-BIKAVESDSA-N
Formula: C31H56N2O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(=NO[Si](C)(C)C)CCC4(C)C3CC(=NO[Si](C)(C)C)C1
Mol. weight [g/mol]: 576.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	8.260		Crippen Method
rinpol	3324.00		NIST Webbook
rinpol	3324.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R215802&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/35-781-6/Methyl-5-beta-cholan-3-12-dione-24-oate-oxime-TMS.pdf>

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