

3-oxo-4,6-chol-24-oate

Other names:	3-oxo-4,6-chol-24-oate, TMS
Inchi:	InChI=1S/C30H50O3Si2/c1-21(10-15-28(31)33-35(7,8)9)25-13-14-26-24-12-11-22-20-23
InchiKey:	QZQZVCPKQMCPPO-UROYWQNLSA-N
Formula:	C30H50O3Si2
SMILES:	CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C=CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C
Mol. weight [g/mol]:	514.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	8.481		Crippen Method
rinqol	3270.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinqol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/97-177-9/3-oxo-4-6-chol-24-oate.pdf>

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