

3-oxo-4,6-chol-24-oate, O-methyloxime (2)

Other names:	3-oxo-4,6-chol-24-oate, O-methyloxime (2), TMS
Inchi:	InChI=1S/C28H45NO3Si/c1-19(8-13-26(30)32-33(5,6)7)23-11-12-24-22-10-9-20-18-21(2)
InchiKey:	JLZQCJFRJSSKLT-BEVKLEDXSA-N
Formula:	C28H45NO3Si
SMILES:	CON=C1C=C2C=CC3C(CCC4(C)C(C(C)CCC(=O)O[Si](C)(C)C)CCC34)C2(C)CC1
Mol. weight [g/mol]:	471.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	7.138		Crippen Method
rinpol	3505.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492361&Units=SI

Legend

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

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<https://www.chemeo.com/cid/56-676-0/3-oxo-4-6-chol-24-oate-O-methyloxime-2.pdf>

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