

3-oxo-4,6-cholesten-26-oate, O-methyloxime-TMS

Other names:	3-oxo-4,6-cholestenoate, O-methyloxime-TMS
Inchi:	InChI=1S/C31H51NO3Si/c1-21(10-9-11-22(2)29(33)35-36(6,7)8)26-14-15-27-25-13-12-2
InchiKey:	RHOOPPMSFUPZJL-YURFGKIPSA-N
Formula:	C31H51NO3Si
SMILES:	CON=C1C=C2C=CC3C(CCC4(C)C(C(C)CCCC(C)C(=O)O[Si](C)(C)C)CCC34)C2(C)CC
Mol. weight [g/mol]:	513.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.31		Crippen Method
logp	8.164		Crippen Method
rinpol	3339.00		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/73-595-1/3-oxo-4-6-cholesten-26-oate-O-methyloxime-TMS.pdf>

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