

7«alpha»-hydroxy-3-oxo-4-chol-24-oate, O-methyloxime, TMS (1)

Inchi: InChI=1S/C31H55NO4Si2/c1-21(11-14-28(33)36-38(8,9)10)24-12-13-25-29-26(16-18-31)
InchiKey: QOTVZIAXEYHVPF-PEXYKONISA-N
Formula: C31H55NO4Si2
SMILES: CON=C1C=C2CC(O[Si](C)(C)C)C3C(CCC4(C)C(C(C)CCC(=O)O[Si](C)(C)C)CCC34)C2
Mol. weight [g/mol]: 561.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	8.192		Crippen Method
rinpol	3250.00		NIST Webbook
rinpol	3265.00		NIST Webbook
rinpol	3250.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R492252&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/50-582-0/7-alpha-hydroxy-3-oxo-4-chol-24-oate-O-methyloxime-TMS-1.pdf>

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