

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

Inchi: InChI=1S/C28H47NO3Si/c1-19(8-13-26(30)32-33(5,6)7)23-11-12-24-22-10-9-20-18-21(2)
InchiKey: GJCWOGDLSUCAKE-BEVKLEDXSA-N
Formula: C28H47NO3Si
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(C)CCC(=O)O[Si](C)(C)C)CCC34)C2(C)CC1
Mol. weight [g/mol]: 473.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	7.362		Crippen Method
rinsol	3362.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R492490&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/115-074-2/3-oxo-4-chol-24-oate-O-methyloxime-TMS-2.pdf>

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