

7«alpha»-hydroxy-3-oxo-4-cholestenoate, oxime-TMS

Inchi: InChI=1S/C36H67NO4Si3/c1-25(15-14-16-26(2)34(38)40-43(8,9)10)29-17-18-30-33-31(2)
InchiKey: AHKBXFYUDFPDIR-BCTRFNONSA-N
Formula: C36H67NO4Si3
SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(=NO[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 662.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	10.424		Crippen Method
rinpol	3280.00		NIST Webbook
rinpol	3280.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R492643&Units=SI>

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/35-771-7/7-alpha-hydroxy-3-oxo-4-cholestenoate-oxime-TMS.pdf>

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