

4-Cholestenoic acid, 7-«beta»-ol-3-one, TMS

Inchi: InChI=1S/C36H66O4Si3/c1-25(15-14-16-26(2)34(37)40-43(11,12)13)29-17-18-30-33-31
InchiKey: OCIWGUDVXZPBDX-VFCGPPIPSA-N
Formula: C36H66O4Si3
SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C)
Mol. weight [g/mol]: 647.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	10.561		Crippen Method
rinpol	3695.00		NIST Webbook
rinpol	3695.00		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=R177478&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/70-643-0/4-Cholestenoic-acid-7-beta-ol-3-one-TMS.pdf>

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