

4-Cholesten-7-«alpha»-ol-3-one, TMS

Other names: 7«alpha»-Hydroxy-4-cholesten-3-one, TMS
7-«alpha»-Hydroxycholest-4-en-3-one, TMS

Inchi: InChI=1S/C33H60O2Si2/c1-23(2)13-12-14-24(3)27-15-16-28-31-29(18-20-33(27,28)5)32

InchiKey: FEHLHHZINBWGES-BJUUDQGOSA-N

Formula: C33H60O2Si2

SMILES: CC(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12

Mol. weight [g/mol]: 545.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	10.203		Crippen Method
rinpol	3230.00		NIST Webbook
rinpol	3200.00		NIST Webbook
rinpol	3210.00		NIST Webbook
rinpol	3210.00		NIST Webbook
rinpol	3230.00		NIST Webbook
rinpol	3235.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R150057&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/65-112-5/4-Cholesten-7-alpha-ol-3-one-TMS.pdf>

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