

Epicholesterol, TMSi (3-O)

Inchi: InChI=1S/C30H56OSi/c1-21(2)10-9-11-22(3)26-14-15-27-25-13-12-23-20-24(31-32(6,7)8)
InchiKey: HRLPEXVPNOBUDF-APWYKTSISA-N
Formula: C30H56OSi
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 460.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	9.328		Crippen Method
rinpol	3044.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R144666&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/60-433-4/Epicholesterol-TMSi-3-O.pdf>

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