

5,6-epoxy-cholesterol, TMS

Inchi: InChI=1S/C30H54O2Si/c1-20(2)10-9-11-21(3)24-12-13-25-23-18-27-30(31-27)19-22(32-27)3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-40
InchiKey: AZHUYKSUWGBLAU-NAZXCJPKSA-N
Formula: C30H54O2Si
SMILES: CC(C)CCCC(C)C1CCC2C3CC4OC45CC(O[Si](C)(C)C)CCC5(C)C3CCC12C
Mol. weight [g/mol]: 474.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.48		Crippen Method
logp	8.459		Crippen Method
rinpol	3209.00		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=R499644&Units=SI>

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.chemeo.com/cid/22-675-8/5-6-epoxy-cholesterol-TMS.pdf>

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