epi-Cholestanol (5«alpha»-cholestan-3«alpha»-ol), TMS

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-OUHAZZKCSA-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	3010.00		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=R435759&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices