8-Dehydrocholesterol, TMS

Inchi: InChI=1S/C29H50OSi/c1-20(2)9-8-10-21(3)27-15-16-28-26-13-11-22-19-23(30-31(5,6)7)

InchiKey: IQCMAKKNYXVJGX-CHCVXNRLSA-N

Formula: C29H50OSi

SMILES: CC(C)CCCC(C)C1CCC2C3=C(CCC21C)C1CCC(O[Si](C)(C)C)CC1=CC3

Mol. weight [g/mol]: 442.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.05		Crippen Method
logp	8.922		Crippen Method
rinpol	3194.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R390968&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices