Zymosterol TMS

Inchi: InChI=1S/C30H52OSi/c1-21(2)10-8-9-11-22(3)28-16-17-29-27-14-12-23-20-24(31-32(5,6
InchiKey: ZCPMAUHTZOMMRX-HHCKZVJDSA-N
Formula: C30H52OSi
SMILES: CC(C)=CCCCC(C)C1CCC2C3=C(CCC21C)C1CCC(O[Si](C)(C)C)CC1CC3
Mol. weight [g/mol]: 456.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.47		Crippen Method
logp	9.312		Crippen Method
rinpol	3178.00		NIST Webbook
rinpol	3178.00		NIST Webbook
rinpol	3178.00		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=R273071&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices