«alpha»-Spinasterol, TMS

Inchi: InChI=1S/C32H56OSi/c1-10-24(22(2)3)12-11-23(4)28-15-16-29-27-14-13-25-21-26(33-3
InchiKey: LBGZUHCDCMFERE-HTUMUVTISA-N
Formula: C32H56OSi
SMILES: CCC(C=CC(C)C1CCC2C3=CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]: 484.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.58		Crippen Method
logp	9.660		Crippen Method
rinpol	3325.00		NIST Webbook
rinpol	3325.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R528668&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