Ergosta-7-en-3«beta»-ol, TMS

Inchi: InChI=1S/C31H56OSi/c1-21(2)22(3)10-11-23(4)27-14-15-28-26-13-12-24-20-25(32-33(7
InchiKey: TVNDUGAVWGGIBH-UHFFFAOYSA-N
Formula: C31H56OSi
SMILES: CC(C)C(C)CCC(C)C1CCC2C3=CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 472.86
CAS: 40272-64-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	9.494		Crippen Method
rinpol	3280.00		NIST Webbook
rinpol	3280.00		NIST Webbook
rinpol	3280.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40272648&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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