cis-Isohumulone, TMS

Inchi: InChI=1S/C29H54O4Si3/c1-21(2)16-17-24-27(30)26(25(20-23(5)6)31-34(7,8)9)28(32-35
InchiKey: XFHXXWFFWSCATK-DJSDQNLUSA-N
Formula: C29H54O4Si3
SMILES: CC(C)=CCC1C(=O)C(C(=CC(C)C)O[Si](C)(C)C)=C(O[Si](C)(C)C)C1(CC=C(C)C)O[Si](C
Mol. weight [g/mol]: 550.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	8.985		Crippen Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		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=R96977&Units=SI

Legend

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