ent-16«beta»,17-H2(OH)2 6«alpha»,7«alpha»(OH)2 kaurenoic acid, MeTMSi

Inchi: InChI=1S/C33H66O6Si4/c1-30-19-16-20-31(2,29(34)35-3)27(30)26(37-41(7,8)9)28(38-42

InchiKey: FTYCAQJYLZNRAF-MDQUFVMMSA-N

Formula: C33H66O6Si4

SMILES: COC(=O)C1(C)CCCC2(C)C1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C13CC(CCC21)C(CO[Si](C

Mol. weight [g/mol]: 671.22

Physical Properties

Property code	Value	Unit	Source
log10ws	0.48		Crippen Method
logp	8.674		Crippen Method
rinpol	2988.00		NIST Webbook
rinpol	2989.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R258498&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