1-Tetrahydrocannabinol, 7-hydroxy, allyl-DMS

Inchi: InChI=1S/C31H50O3Si2/c1-11-14-15-16-24-21-26-29(27(22-24)33-35(7,8)17-12-2)25-19
InchiKey: FVFYFUKUXCZGNP-JETRDCLMSA-N
Formula: C31H50O3Si2
SMILES: C=CC[Si](C)(C)Oc1cc(CCCCC)cc2c1C1C=C(C)CC(O[Si](C)(C)CC=C)C1C(C)(C)O2
Mol. weight [g/mol]: 526.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.76		Crippen Method
logp	9.186		Crippen Method
rinpol	2936.00		NIST Webbook
rinpol	2936.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525976&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