1-Tetrahydrocannabinol, 6«alpha»-hydroxy, allyl-DMS

Inchi: InChI=1S/C31H50O3Si2/c1-11-14-15-16-25-22-27-29(28(23-25)33-35(7,8)19-12-2)26-21

InchiKey: VPMAHVULICCGNE-NEEKEDPPSA-N

Formula: C31H50O3Si2

SMILES: C=CC[Si](C)(C)Oc1cc(CCCCC)cc2c1C1C=C(C)CCC1(O[Si](C)(C)CC=C)C(C)(C)O2

Mol. weight [g/mol]: 526.90

Physical Properties

Property code	Value	Unit	Source
logp	9.330		Crippen Method
rinpol	2915.00		NIST Webbook
rinpol	2915.00		NIST Webbook

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525941&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices