

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

Latest version available from:

<https://www.chemeo.com/cid/119-974-9/1-Tetrahydrocannabinol-6-alpha-hydroxy-allyl-DMS.pdf>

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