Cannabidiol, allyl-DMS

Inchi: InChI=1S/C31H50O2Si2/c1-11-14-15-16-26-22-29(32-34(7,8)19-12-2)31(30(23-26)33-35
InchiKey: LQVLXLSBZAMCKD-QXPUDEPPSA-N
Formula: C31H50O2Si2
SMILES: C=CC[Si](C)(C)Oc1cc(CCCCC)cc(O[Si](C)(C)CC=C)c1C1C=C(C)CCC1C(=C)C
Mol. weight [g/mol]: 510.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	9.975		Crippen Method
rinpol	2565.00		NIST Webbook
rinpol	2565.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R526355&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