1-Tetrahydrocannabinol, allyl-DMS

Inchi: InChI=1S/C26H40O2Si/c1-8-10-11-12-20-17-23-25(24(18-20)28-29(6,7)15-9-2)21-16-19
InchiKey: ONMWMOCWZMNKAH-VXKWHMMOSA-N
Formula: C26H40O2Si
SMILES: C=CC[Si](C)(C)Oc1cc(CCCCC)cc2c1C1C=C(C)CCC1C(C)(C)O2
Mol. weight [g/mol]: 412.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.56		Crippen Method
logp	7.800		Crippen Method
rinpol	2514.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R526008&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices