1-Tetrahydrocannabinol, 7-hydroxy, TBDMS

Inchi: InChI=1S/C33H58O3Si2/c1-15-16-17-18-24-21-26-29(27(22-24)35-37(11,12)31(3,4)5)25
InchiKey: NJYOJCSBHZZTCW-JETRDCLMSA-N
Formula: C33H58O3Si2
SMILES: CCCCCc1cc2c(c(O[Si](C)(C)C(C)(C)C)c1)C1C=C(C)CC(O[Si](C)(C)C(C)(C)C)C1C(C)(C
Mol. weight [g/mol]: 558.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.89		Crippen Method
logp	10.414		Crippen Method
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525981&Units=SI

Legend

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