1-Tetrahydrocannabinol, TBDMS

Inchi: InChI=1S/C27H44O2Si/c1-10-11-12-13-20-17-23-25(24(18-20)29-30(8,9)26(3,4)5)21-16-
InchiKey: JLRFZWKTGGRERL-VXKWHMMOSA-N
Formula: C27H44O2Si
SMILES: CCCCCc1cc2c(c(O[Si](C)(C)C(C)(C)C)c1)C1C=C(C)CCC1C(C)(C)O2
Mol. weight [g/mol]: 428.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	8.414		Crippen Method
rinpol	2560.00		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=R526013&Units=SI

Legend

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