Cannabidiol di-tms derivative

Other names: Cannabidiol, TMS
Inchi: InChI=1S/C27H46O2Si2/c1-11-12-13-14-22-18-25(28-30(5,6)7)27(26(19-22)29-31(8,9)10
InchiKey: FWZOFSHJDAIJQE-UHFFFAOYSA-N
Formula: C27H46O2Si2
SMILES: C=C(C)C1CCC(C)=CC1c1c(O[Si](C)(C)C)cc(CCCCC)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 458.82
CAS: 64846-15-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	8.863		Crippen Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64846157&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