1-Tetrahydrocannabinol, 6«alpha»-hydroxy, TMS

Inchi: InChI=1S/C27H46O3Si2/c1-11-12-13-14-21-18-23-25(24(19-21)29-31(5,6)7)22-17-20(2)

InchiKey: MJSIMUXAYFZIQN-AMGIVPHBSA-N

Formula: C27H46O3Si2

SMILES: CCCCCc1cc2c(c(O[Si](C)(C)C)c1)C1C=C(C)CCC1(O[Si](C)(C)C)C(C)(C)O2

Mol. weight [g/mol]: 474.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	8.218		Crippen Method
rinpol	2580.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525961&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

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