6-Tetrahydrocannabinol, TMS

Inchi: InChI=1S/C24H38O2Si/c1-8-9-10-11-18-15-21-23(22(16-18)26-27(5,6)7)19-14-17(2)12-1
InchiKey: SHMIIDWJPSMGBP-PMACEKPBSA-N
Formula: C24H38O2Si
SMILES: CCCCCc1cc2c(c(O[Si](C)(C)C)c1)C1CC(C)=CCC1C(C)(C)O2
Mol. weight [g/mol]: 386.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	7.244		Crippen Method
rinpol	2335.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R526340&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