Propyl-1-tetrahydrocannabinol, TBDMS

Inchi: InChI=1S/C25H40O2Si/c1-10-11-18-15-21-23(22(16-18)27-28(8,9)24(3,4)5)19-14-17(2)1
InchiKey: VGZKQUKIOPZBOU-GFOWMXPYSA-N
Formula: C25H40O2Si
SMILES: CCCc1cc2c(c(O[Si](C)(C)C(C)(C)C)c1)C1C=C(C)CCC1C(C)(C)O2
Mol. weight [g/mol]: 400.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.29		Crippen Method
logp	7.634		Crippen Method
rinpol	2385.00		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=R526459&Units=SI

Legend

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