cannabinolic acid, TMS

Inchi: InChI=1S/C28H42O4Si2/c1-11-12-13-14-20-18-23-25(21-17-19(2)15-16-22(21)28(3,4)30
InchiKey: VMNPNZRMQWEPIJ-UHFFFAOYSA-N
Formula: C28H42O4Si2
SMILES: CCCCCc1cc2c(c(O[Si](C)(C)C)c1C(=O)O[Si](C)(C)C)-c1cc(C)ccc1C(C)(C)O2
Mol. weight [g/mol]: 498.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.73		Crippen Method
logp	8.228		Crippen Method
rinpol	2743.00		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=R487582&Units=SI

Legend

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