Obtusifolin, TMS

Inchi: InChI=1S/C22H28O5Si2/c1-13-12-15-18(22(25-2)21(13)27-29(6,7)8)20(24)17-14(19(15)
InchiKey: AUBMEVJELBUQSK-UHFFFAOYSA-N
Formula: C22H28O5Si2
SMILES: COc1c(O[Si](C)(C)C)c(C)cc2c1C(=O)c1c(O[Si](C)(C)C)cccc1C2=O
Mol. weight [g/mol]: 428.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	5.206		Crippen Method
rinpol	2737.00		NIST Webbook
rinpol	2737.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R158264&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