5-Caffeoyl quinic acid, TMS

Inchi: InChI=1S/C35H68O9Si6/c1-45(2,3)39-28-23-22-27(24-29(28)40-46(4,5)6)20-19-21-32(3
InchiKey: HPWKLMNWHGHVHX-SZHIFFBKSA-N
Formula: C35H68O9Si6
SMILES: C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(OC(=O)CC=Cc2ccc(O[Si](C)(C)C)c(O[Si](C)(C)C
Mol. weight [g/mol]: 801.42

Physical Properties

Property code	Value	Unit	Source
log10ws	3.37		Crippen Method
logp	9.632		Crippen Method
rinpol	3190.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R507027&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