3-Caffeoyl quinic acid, TMS

Inchi: InChI=1S/C34H66O9Si6/c1-44(2,3)38-27-21-19-26(23-28(27)39-45(4,5)6)20-22-31(35)3
InchiKey: ZUMPKHAQJVFOSF-XDUBOXGASA-N
Formula: C34H66O9Si6
SMILES: C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(OC(=O)C=Cc2ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)
Mol. weight [g/mol]: 787.40

Physical Properties

Property code	Value	Unit	Source
log10ws	3.78		Crippen Method
logp	9.241		Crippen Method
rinpol	3113.70		NIST Webbook
rinpol	3113.70		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R507012&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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