4-Caffeoyl quinic acid, TMS

Inchi: InChI=1S/C32H64O9Si6/c1-42(2,3)36-25-20-19-24(21-26(25)37-43(4,5)6)30(33)35-29-2

InchiKey: AJOSHXXJFGXQEX-UHFFFAOYSA-N

Formula: C32H64O9Si6

SMILES: C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C(OC(=O)c2ccc(O[Si](C)(C)C)c(O[

Mol. weight [g/mol]: 761.36

Physical Properties

Property code	Value	Unit	Source
log10ws	4.07		Crippen Method
logp	8.842		Crippen Method
rinpol	3168.30		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=R241688&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

https://www.chemeo.com/cid/46-802-0/4-Caffeoyl-quinic-acid-TMS.pdf