

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(30-31)18-17-16-15-14-13-12-11-10-9-8-7-6-5-4-3-2-1
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)O2
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/ci9903071>

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/38-687-8/5-Caffeoyl-quinic-acid-TMS.pdf>

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