trans-3-O-Coumaroyl-D-quinic acid, pentakis-TMS

Inchi: InChI=1S/C31H58O8Si5/c1-40(2,3)35-25-19-16-24(17-20-25)18-21-28(32)34-26-22-31(3

InchiKey: NJXINYMXFRUJJM-NBAWZLICSA-N

Formula: C31H58O8Si5

SMILES: C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(OC(=O)C=Cc2ccc(O[Si](C)(C)C)cc2)C(O[Si](C)(

Mol. weight [g/mol]: 699.21

Physical Properties

Property code	Value	Unit	Source
log10ws	2.79		Crippen Method
logp	8.028		Crippen Method
rinpol	3110.00		NIST Webbook
rinpol	3110.00		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=R599729&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices