

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)(C)C)C1
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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/119-975-8/trans-3-O-Coumaroyl-D-quinic-acid-pentakis-TMS.pdf>

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