

3-O-Coumaroyl-D-quinic acid, 5TMS

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-DYTRJAOYSA-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
CAS: 179465-94-2

Physical Properties

Property code	Value	Unit	Source
log10ws	2.79		Crippen Method
logp	8.028		Crippen Method
rinpol	3048.00		NIST Webbook
rinpol	2962.10		NIST Webbook
rinpol	2962.10		NIST Webbook
rinpol	3048.00		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=C179231120&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/116-689-9/3-O-Coumaroyl-D-quinic-acid-5TMS.pdf>

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