

1-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)35-32(34)31-22-23-24
InchiKey: ABQAILCNIKFUPS-UHFFFAOYSA-N
Formula: C32H64O9Si6
SMILES: C[Si](C)(C)OC(=O)C1(OC(=O)c2ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c2)CC(O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 761.36

Physical Properties

Property code	Value	Unit	Source
log10ws	4.07		Crippen Method
logp	8.842		Crippen Method
rinpol	3397.00		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=R241668&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/24-696-3/1-Caffeoyl-quinic-acid-TMS.pdf>

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