

Caffeoylquinic acid, 4-trans-, 6TMS

Inchi: InChI=1S/C34H66O9Si6/c1-44(2,3)38-27-21-19-26(23-28(27)39-45(4,5)6)20-22-31(35)3
InchiKey: TVNYJEUSYBSSPM-UYAFOJL TSA-N
Formula: C34H66O9Si6
SMILES: C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C(OC(=O)C=Cc2ccc(O[Si](C)(C)C)C2
Mol. weight [g/mol]: 787.40

Physical Properties

Property code	Value	Unit	Source
log10ws	3.78		Crippen Method
logp	9.241		Crippen Method
rinpol	3189.00		NIST Webbook
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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=R605597&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/117-119-0/Caffeoylquinic-acid-4-trans-6TMS.pdf>

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