

3-O-Feruloylquinic acid, 5TMS

Inchi: InChI=1S/C32H60O9Si5/c1-35-26-21-24(17-19-25(26)37-42(2,3)4)18-20-29(33)36-27-22
InchiKey: IXVPJAVYTLDRIA-CZIZESTLSA-N
Formula: C32H60O9Si5
SMILES: COc1cc(C=CC(=O)OC2CC(O[Si](C)(C)C)(C(=O)O[Si](C)(C)C)CC(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]: 729.24

Physical Properties

Property code	Value	Unit	Source
log10ws	2.67		Crippen Method
logp	8.036		Crippen Method
rinsol	3162.10		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U414051&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/114-921-2/3-O-Feruloylquinic-acid-5TMS.pdf>

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