4-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)36-30-27
InchiKey: BEQVWSBUEPSOFX-CZIZESTLSA-N
Formula: C32H60O9Si5
SMILES: COc1cc(C=CC(=O)OC2C(O[Si](C)(C)C)CC(O[Si](C)(C)C)(C(=O)O[Si](C)(C)C)CC2O[Si](
Mol. weight [g/mol]: 729.24

Physical Properties

Property code	Value	Unit	Source
log10ws	2.67		Crippen Method
logp	8.036		Crippen Method
rinpol	3137.50		NIST Webbook
rinpol	3137.50		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=U414046&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/115-119-2/4-O-Feruloylquinic-acid-5TMS.pdf
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