2-Phenylethyl (E)-isoferulate, TMS

Inchi: InChI=1S/C21H26O4Si/c1-23-19-12-10-18(16-20(19)25-26(2,3)4)11-13-21(22)24-15-14-
InchiKey: MZMONAFSPJMFIP-ACCUITESSA-N
Formula: C21H26O4Si
SMILES: COc1ccc(C=CC(=O)OCCc2ccccc2)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 370.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	4.708		Crippen Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R42219&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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