Benzyl (Z)-isoferulate, TMS

Inchi: InChI=1S/C20H24O4Si/c1-22-18-12-10-16(14-19(18)24-25(2,3)4)11-13-20(21)23-15-17-8
InchiKey: BSQMZKMLQHRBCC-QBFSEMIESA-N
Formula: C20H24O4Si
SMILES: COc1ccc(C=CC(=O)OCc2ccccc2)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 356.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	4.665		Crippen Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R42291&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