2-Methylpropyl (E)-isoferulate, TMS

Inchi: InChI=1S/C17H26O4Si/c1-13(2)12-20-17(18)10-8-14-7-9-15(19-3)16(11-14)21-22(4,5)6/
InchiKey: QCUKNNMYAGJGQQ-CSKARUKUSA-N
Formula: C17H26O4Si
SMILES: COc1ccc(C=CC(=O)OCC(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	4.121		Crippen Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R42198&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