2-Methyl-2-propenyl (E)-isoferulate, TMS

Inchi: InChI=1S/C17H24O4Si/c1-13(2)12-20-17(18)10-8-14-7-9-15(19-3)16(11-14)21-22(4,5)6/
InchiKey: GRUNAUVVSMPNLW-CSKARUKUSA-N
Formula: C17H24O4Si
SMILES: C=C(C)COC(=O)C=Cc1ccc(OC)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 320.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	4.041		Crippen Method
rinpol	2167.00		NIST Webbook
rinpol	2167.00		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=R42170&Units=SI

Legend

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