2-Nethyl-3-butenyl (Z)-isoferulate, TMS

Inchi: InChI=1S/C18H26O4Si/c1-7-14(2)13-21-18(19)11-9-15-8-10-16(20-3)17(12-15)22-23(4,5
InchiKey: IOQNHVPGRZIWSO-PKNBQFBNSA-N
Formula: C18H26O4Si
SMILES: C=CC(C)COC(=O)C=Cc1ccc(OC)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 334.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	4.287		Crippen Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R42205&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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