2-Methyl-2-butenyl (E)-4-acetylcaffeate, TMS

Inchi: InChI=1S/C19H26O5Si/c1-7-14(2)13-22-19(21)11-9-16-8-10-17(23-15(3)20)18(12-16)24
InchiKey: VUGYZKVMAHRHLU-FRVKRSESSA-N
Formula: C19H26O5Si
SMILES: CC=C(C)COC(=O)C=Cc1ccc(OC(C)=O)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 362.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	4.348		Crippen Method
rinpol	2388.00		NIST Webbook
rinpol	2388.00		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=R173010&Units=SI

Legend

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