3-Methyl-3-butenyl (E)-4-acetylcaffeate, TMS

Inchi: InChI=1S/C19H26O5Si/c1-14(2)11-12-22-19(21)10-8-16-7-9-17(23-15(3)20)18(13-16)24
InchiKey: MTZTYCNIBLXYIG-CSKARUKUSA-N
Formula: C19H26O5Si
SMILES: C=C(C)CCOC(=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	2352.00		NIST Webbook
rinpol	2352.00		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=R173090&Units=SI

Legend

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