

# 2-Methyl-2-butenyl (E)-3-acetylcaffeate, TMS

**Inchi:** InChI=1S/C19H26O5Si/c1-7-14(2)13-22-19(21)11-9-16-8-10-17(24-25(4,5)6)18(12-16)23  
**InchiKey:** IPPNDQQSCOSGEL-FRVKRSESSA-N  
**Formula:** C19H26O5Si  
**SMILES:** CC=C(C)COC(=O)C=Cc1ccc(O[Si](C)(C)C)c(OC(C)=O)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	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R173005&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

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