

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

**Inchi:** InChI=1S/C19H26O5Si/c1-14(2)11-12-22-19(21)10-8-16-7-9-17(24-25(4,5)6)18(13-16)23  
**InchiKey:** NXRJJFYGGQYRJDU-CSKARUKUSA-N  
**Formula:** C19H26O5Si  
**SMILES:** C=C(C)CCOC(=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	2417.00		NIST Webbook
rinpol	2417.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R173085&Units=SI>

## Legend

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

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