

# 3-Methyl-2-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:** BUOUKBLUZBRGLM-CSKARUKUSA-N  
**Formula:** C19H26O5Si  
**SMILES:** CC(=O)Oc1ccc(C=CC(=O)OCC=C(C)C)cc1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 362.49

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.84   |      | Crippen Method |
| logp          | 4.348   |      | Crippen Method |
| rinpol        | 2398.00 |      | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R173065&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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