# 2-Phenylethyl (E)-3-acetylcaffeate, TMS

**Inchi:** InChI=1S/C22H26O5Si/c1-17(23)26-21-16-19(10-12-20(21)27-28(2,3)4)11-13-22(24)25-
**InchiKey:** JLGGKGJZXSCANR-ACCUITESSA-N
**Formula:** C22H26O5Si
**SMILES:** CC(=O)Oc1cc(C=CC(=O)OCCc2ccccc2)ccc1O[Si](C)(C)C
**Mol. weight [g/mol]:** 398.52

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.35 | | Crippen Method |
| logp | 4.625 | | Crippen Method |
| rinpol | 2844.00 | | NIST Webbook |

## Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R173025&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

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