

# Benzyl (E)-4-acetylcaffeate, TMS

**Inchi:** InChI=1S/C21H24O5Si/c1-16(22)25-19-12-10-17(14-20(19)26-27(2,3)4)11-13-21(23)24-  
**InchiKey:** OBWFWGYXOQUFEK-ACCUITESSA-N  
**Formula:** C21H24O5Si  
**SMILES:** CC(=O)Oc1ccc(C=CC(=O)OCc2ccccc2)cc1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 384.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	4.582		Crippen Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook

## Sources

**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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R173129&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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<https://www.chemeo.com/cid/96-305-7/Benzyl-E-4-acetylcaffeate-TMS.pdf>

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