

# 2-Phenylethyl (E)-isoferulate, TMS

**Inchi:** InChI=1S/C21H26O4Si/c1-23-19-12-10-18(16-20(19)25-26(2,3)4)11-13-21(22)24-15-14-  
**InchiKey:** MZMONAFSPJMFIP-ACCUITESSA-N  
**Formula:** C<sub>21</sub>H<sub>26</sub>O<sub>4</sub>Si  
**SMILES:** COc1ccc(C=CC(=O)OCCc2ccccc2)cc1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 370.51

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	4.708		Crippen Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R42219&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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<https://www.chemeo.com/cid/70-853-7/2-Phenylethyl-E-isoferulate-TMS.pdf>

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