

# 3-Methylbutyl (E)-isoferulate, TMS

**Inchi:** InChI=1S/C18H28O4Si/c1-14(2)11-12-21-18(19)10-8-15-7-9-16(20-3)17(13-15)22-23(4,5)  
**InchiKey:** MOFQCEGVUYCISG-CSKARUKUSA-N  
**Formula:** C18H28O4Si  
**SMILES:** COc1ccc(C=CC(=O)OCCC(C)C)cc1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 336.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	4.511		Crippen Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R42273&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

Latest version available from:

<https://www.cheméo.com/cid/64-101-8/3-Methylbutyl-E-isoferulate-TMS.pdf>

Generated by Cheméo on 2024-04-20 05:37:00.360342972 +0000 UTC m=+15880669.280920287.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.