

# 3-Phenylbutyric acid, TBDMS

**Inchi:** InChI=1S/C16H26O2Si/c1-13(14-10-8-7-9-11-14)12-15(17)18-19(5,6)16(2,3)4/h7-11,13H  
**InchiKey:** JDKNNBZVVUJDRI-UHFFFAOYSA-N  
**Formula:** C16H26O2Si  
**SMILES:** CC(CC(=O)O[Si](C)(C)C(C)(C)C)c1ccccc1  
**Mol. weight [g/mol]:** 278.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	4.729		Crippen Method
rinpol	1677.00		NIST Webbook

## Sources

**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=R563601&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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/15-452-3/3-Phenylbutyric-acid-TBDMS.pdf>

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