

# (.+/-.)-2-Phenylbutyric acid, tert-butyldimethylsilyl ester

**Other names:** tert-Butyl(dimethyl)silyl 2-phenylbutanoate

2-Phenylbutyric acid, TBDMS

2-Phenylbutyric acid, tbdms derivative

**Inchi:** InChI=1S/C16H26O2Si/c1-7-14(13-11-9-8-10-12-13)15(17)18-19(5,6)16(2,3)4/h8-12,14H

**InchiKey:** IWSNKTSLOBHITP-UHFFFAOYSA-N

**Formula:** C16H26O2Si

**SMILES:** CCC(C(=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	1600.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1602.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333146&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

Latest version available from:

<https://www.chemeo.com/cid/47-653-5/2-Phenylbutyric-acid-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-29 13:22:01.616485827 +0000 UTC m=+16686170.537063140.

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