

# Benzenepropanoic acid, «alpha»-[(tert-butyldimethylsilyl)oxy]-, tert-butyldimethylsilyl ester

Other names: DL-3-Phenylactic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester  
3-Phenylactic acid, TBDMS

Phenylactic acid, TBDMS

**Inchi:** InChI=1S/C21H38O3Si2/c1-20(2,3)25(7,8)23-18(16-17-14-12-11-13-15-17)19(22)24-26(27,28)  
**InchiKey:** JFLMDZUHGCHDPN-UHFFFAOYSA-N  
**Formula:** C21H38O3Si2  
**SMILES:** CC(C)(C)[Si](C)(C)OC(=O)C(Cc1ccccc1)O[Si](C)(C)C(C)(C)C  
**Mol. weight [g/mol]:** 394.70  
**CAS:** 89682-03-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	6.168		Crippen Method
rinpol	2031.10		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2016.00		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=C89682031&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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