

# Phenylpyruvic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester

**Other names:** Phenylpyruvic acid, DMTBS  
Phenylpyruvic acid, TBDMS

**Inchi:** InChI=1S/C21H36O3Si2/c1-20(2,3)25(7,8)23-18(16-17-14-12-11-13-15-17)19(22)24-26(

**InchiKey:** RMGPQKOYNWVGPE-VLGSPTGOSA-N

**Formula:** C21H36O3Si2

**SMILES:** CC(C)(C)[Si](C)(C)OC(=O)C(=Cc1ccccc1)O[Si](C)(C)C(C)(C)C

**Mol. weight [g/mol]:** 392.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	6.598		Crippen Method
rinpol	2104.00		NIST Webbook
rinpol	2125.70		NIST Webbook
rinpol	2125.70		NIST Webbook
rinpol	2104.00		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=U352582&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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