

# Phenylpropionylglycine, TMS # 1

**Inchi:** InChI=1S/C14H21NO3Si/c1-5-13(16)15(12-9-7-6-8-10-12)11-14(17)18-19(2,3)4/h6-10H,  
**InchiKey:** ZAGVQHZEJKLQHM-UHFFFAOYSA-N  
**Formula:** C14H21NO3Si  
**SMILES:** CCC(=O)N(CC(=O)O[Si](C)(C)C)c1ccccc1  
**Mol. weight [g/mol]:** 279.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.58		Crippen Method
logp	2.808		Crippen Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R401380&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

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