

# Phenylphosphonic acid, ethyl tridecyl ester

**Inchi:** InChI=1S/C21H37O3P/c1-3-5-6-7-8-9-10-11-12-13-17-20-24-25(22,23-4-2)21-18-15-14-  
**InchiKey:** WAUJYSIVRUSYTO-UHFFFAOYSA-N  
**Formula:** C21H37O3P  
**SMILES:** CCCCCCCCCCCCOP(=O)(OCC)c1ccccc1  
**Mol. weight [g/mol]:** 368.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.55		Crippen Method
logp	6.869		Crippen Method
mcvol	321.060	ml/mol	McGowan Method
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393251&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  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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