

# Phenylphosphonic acid, 2,4,4-trimethylpentyl nonyl ester

**Inchi:** InChI=1S/C23H41O3P/c1-6-7-8-9-10-11-15-18-25-27(24,22-16-13-12-14-17-22)26-20-21  
**InchiKey:** XYGCAEGLJAVAFC-UHFFFAOYSA-N  
**Formula:** C23H41O3P  
**SMILES:** CCCCCCCCOP(=O)(OCC(C)CC(C)(C)C)c1cccc1  
**Mol. weight [g/mol]:** 396.54

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.90		Crippen Method
logp	7.361		Crippen Method
mcvol	349.240	ml/mol	McGowan Method
rinpol	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393224&Units=SI>

## 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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