

# Phenylphosphonic acid, dodecyl hexyl ester

**Inchi:** InChI=1S/C24H43O3P/c1-3-5-7-9-10-11-12-13-14-19-23-27-28(25,24-20-16-15-17-21-24)  
**InchiKey:** VVXCOIHS AIBOHO-UHFFFAOYSA-N  
**Formula:** C<sub>24</sub>H<sub>43</sub>O<sub>3</sub>P  
**SMILES:** CCCCCCCCCCOP(=O)(OCCCCC)c1ccccc1  
**Mol. weight [g/mol]:** 410.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-13.81		Crippen Method
logp	8.039		Crippen Method
mcvol	363.330	ml/mol	McGowan Method
rinpol	2875.00		NIST Webbook
rinpol	2875.00		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=U393244&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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