

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

**Inchi:** InChI=1S/C24H43O3P/c1-6-7-8-9-10-11-12-16-19-26-28(25,23-17-14-13-15-18-23)27-21  
**InchiKey:** MPSJHUAVOVOWQZ-UHFFFAOYSA-N  
**Formula:** C24H43O3P  
**SMILES:** CCCCCCCCCOP(=O)(OCC(C)CC(C)(C)C)c1cccc1  
**Mol. weight [g/mol]:** 410.57

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -13.32  |        | Crippen Method |
| logp          | 7.751   |        | Crippen Method |
| mcvol         | 363.330 | ml/mol | McGowan Method |
| rinpol        | 2689.00 |        | NIST Webbook   |
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## 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=U393225&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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