

# Phenylphosphonic acid, dodecyl octyl ester

**Inchi:** InChI=1S/C26H47O3P/c1-3-5-7-9-11-12-13-14-16-21-25-29-30(27,26-22-18-17-19-23-26)  
**InchiKey:** ZSSDAERINUPIJA-UHFFFAOYSA-N  
**Formula:** C26H47O3P  
**SMILES:** CCCCCCCCCCOP(=O)(OCCCCCCCC)c1ccccc1  
**Mol. weight [g/mol]:** 438.62

## Physical Properties

Property code	Value	Unit	Source
log10ws	-14.64		Crippen Method
logp	8.820		Crippen Method
mcvol	391.510	ml/mol	McGowan Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393246&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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