

# Bis(3,5-dimethylphenyl)-2-ethyl-4-methylpentyl phosphate

**InChI:** InChI=1S/C24H35O4P/c1-8-22(9-17(2)3)16-26-29(25,27-23-12-18(4)10-19(5)13-23)28-2  
**InChIKey:** SNMYVUCYGMKUPF-UHFFFAOYSA-N  
**Formula:** C24H35O4P  
**SMILES:** CCC(COP(=O)(Oc1cc(C)cc(C)c1)Oc1cc(C)cc(C)c1)CC(C)C  
**Mol. weight [g/mol]:** 418.51  
**CAS:** 116402-05-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.64		Crippen Method
logp	7.575		Crippen Method
mcvol	345.440	ml/mol	McGowan Method

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402052&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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