

# Dimethyl 3-methylphenyl phosphate

**Inchi:** InChI=1S/C9H13O4P/c1-8-5-4-6-9(7-8)13-14(10,11-2)12-3/h4-7H,1-3H3  
**InchiKey:** BQGIVCKQWCUOME-UHFFFAOYSA-N  
**Formula:** C9H13O4P  
**SMILES:** COP(=O)(OC)Oc1cccc(C)c1  
**Mol. weight [g/mol]:** 216.17

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	2.775		Crippen Method
mcvol	157.850	ml/mol	McGowan Method
rinpol	1488.00		NIST Webbook
ripol	2219.00		NIST Webbook

## 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=R168999&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  
**rinpol:** Non-polar retention indices  
**ripol:** Polar retention indices

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