

# Dibutyl 3-chloro-phenyl phosphate

**Inchi:** InChI=1S/C14H22ClO4P/c1-3-5-10-17-20(16,18-11-6-4-2)19-14-9-7-8-13(15)12-14/h7-9,  
**InchiKey:** RKAOVMNICNPHMW-UHFFFAOYSA-N  
**Formula:** C14H22ClO4P  
**SMILES:** CCCCOP(=O)(OCCCC)Oc1cccc(Cl)c1  
**Mol. weight [g/mol]:** 320.75

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	5.460		Crippen Method
mcvol	240.540	ml/mol	McGowan Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook
ripol	2730.00		NIST Webbook
ripol	2730.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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=R168815&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  
**ripol:** Polar retention indices

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