

# Dimethyl 3-cyano-phenyl phosphate

**Inchi:** InChI=1S/C9H10NO4P/c1-12-15(11,13-2)14-9-5-3-4-8(6-9)7-10/h3-6H,1-2H3  
**InchiKey:** KAOVBKCOGJNYGW-UHFFFAOYSA-N  
**Formula:** C9H10NO4P  
**SMILES:** COP(=O)(OC)Oc1cccc(C#N)c1  
**Mol. weight [g/mol]:** 227.15

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	2.338		Crippen Method
mcvol	159.230	ml/mol	McGowan Method
rinpole	1678.00		NIST Webbook
ripole	2625.00		NIST Webbook
ripol	2625.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R168984&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307i>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices  
**ripole:** Polar retention indices

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