

# Dibutyl 4-nitro-phenyl phosphate

**Other names:** Paraoxon butyl  
**Inchi:** InChI=1S/C14H22NO6P/c1-3-5-11-19-22(18,20-12-6-4-2)21-14-9-7-13(8-10-14)15(16)17  
**InchiKey:** CKVWBMJDISUJJM-UHFFFAOYSA-N  
**Formula:** C14H22NO6P  
**SMILES:** CCCCOP(=O)(OCCCC)Oc1ccc([N+](=O)[O-])cc1  
**Mol. weight [g/mol]:** 331.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.61		Crippen Method
logp	4.715		Crippen Method
mcvol	245.720	ml/mol	McGowan Method
rinpol	2345.00		NIST Webbook
ripol	3180.00		NIST Webbook
ripol	3180.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R5124&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)

## 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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