

# Isoxathion oxon

**Inchi:** InChI=1S/C13H16NO5P/c1-3-16-20(15,17-4-2)19-13-10-12(18-14-13)11-8-6-5-7-9-11/h5  
**InchiKey:** VLBRWDJSOHOVGF-UHFFFAOYSA-N  
**Formula:** C13H16NO5P  
**SMILES:** CCOP(=O)(OCC)Oc1cc(-c2ccccc2)on1  
**Mol. weight [g/mol]:** 297.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.39		Crippen Method
logp	3.901		Crippen Method
mcvol	210.600	ml/mol	McGowan Method
rinpol	2169.00		NIST Webbook
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R197521&Units=SI>  
**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)

## Legend

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

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