

# Phosphoric acid, tris(2,2-dimethylpentyl) ester

**Inchi:** InChI=1S/C21H45O4P/c1-10-13-19(4,5)16-23-26(22,24-17-20(6,7)14-11-2)25-18-21(8,9)  
**InchiKey:** WEDRSNCKSZVNAJ-UHFFFAOYSA-N  
**Formula:** C21H45O4P  
**SMILES:** CCCC(C)(C)COP(=O)(OCC(C)(C)CCC)OCC(C)(C)CCC  
**Mol. weight [g/mol]:** 392.55  
**CAS:** 116402-18-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.41		Crippen Method
logp	7.623		Crippen Method
mcvol	350.690	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402187&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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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