

# Phosphoric acid, trihexyl ester

**Inchi:** InChI=1S/C18H39O4P/c1-4-7-10-13-16-20-23(19,21-17-14-11-8-5-2)22-18-15-12-9-6-3/H  
**InchiKey:** SFENPMLASUEABX-UHFFFAOYSA-N  
**Formula:** C18H39O4P  
**SMILES:** CCCCCCOP(=O)(OCCCCC)OCCCCC  
**Mol. weight [g/mol]:** 350.47

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.88		Crippen Method
logp	6.885		Crippen Method
mcvol	308.420	ml/mol	McGowan Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308911&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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