

# Methylthiophosphonic acid, O-ethyl, S-(8-diisopropylamino)-1,3,6-trithiaoctyl ester

**Inchi:** InChI=1S/C14H32NO2PS4/c1-7-17-18(6,16)22-21-12-20-11-10-19-9-8-15(13(2)3)14(4)5  
**InchiKey:** XFIORCMIGKMUNX-UHFFFAOYSA-N  
**Formula:** C14H32NO2PS4  
**SMILES:** CCOP(C)(=O)SSCSCCSCCN(C(C)C)C(C)C  
**Mol. weight [g/mol]:** 405.64

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.86		Crippen Method
logp	5.770		Crippen Method
mcvol	315.700	ml/mol	McGowan Method
rinpol	2628.00		NIST Webbook
rinpol	2628.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R338539&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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  
**rinpol:** Non-polar retention indices

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