

# Methylthiophosphonic acid, O,O-diisobutyl ester

**Inchi:** InChI=1S/C9H21O2PS/c1-8(2)6-10-12(5,13)11-7-9(3)4/h8-9H,6-7H2,1-5H3  
**InchiKey:** CGQXFKONQUGVCM-UHFFFAOYSA-N  
**Formula:** C9H21O2PS  
**SMILES:** CC(C)COP(C)(=S)OCC(C)C  
**Mol. weight [g/mol]:** 224.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.46		Crippen Method
logp	3.271		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
rinpol	1331.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1331.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R334928&Units=SI>

## 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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