

# O-(4-methylphenyl) dichloridothiophosphate

<b>Inchi:</b>	InChI=1S/C7H7Cl2OPS/c1-6-2-4-7(5-3-6)10-11(8,9)12/h2-5H,1H3
<b>InchiKey:</b>	RDGYPSHBQMWDHX-UHFFFAOYSA-N
<b>Formula:</b>	C7H7Cl2OPS
<b>SMILES:</b>	Cc1ccc(OP(=S)(Cl)Cl)cc1
<b>Mol. weight [g/mol]:</b>	241.07
<b>CAS:</b>	18961-95-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.21		Crippen Method
logp	4.076		Crippen Method
mcvol	152.890	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C18961950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18961950&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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<https://www.chemeo.com/cid/28-756-2/O-4-methylphenyl-dichloridothiophosphate.pdf>

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