

# O-methyl o-(2,4,6-trichlorophenyl)amidothiophosphate

<b>Inchi:</b>	InChI=1S/C7H7Cl3NO2PS/c1-12-14(11,15)13-7-5(9)2-4(8)3-6(7)10/h2-3H,1H3,(H2,11,15)
<b>InchiKey:</b>	DKSPJOUWMRFPD-UHFFFAOYSA-N
<b>Formula:</b>	C7H7Cl3NO2PS
<b>SMILES:</b>	COP(N)(=S)Oc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	306.53
<b>CAS:</b>	116401-96-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	3.855		Crippen Method
mcvol	180.980	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=C116401968&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401968&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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