

# O-ethyl o-(2,4,5-trichlorophenyl) methylamidothiophosphate

<b>Inchi:</b>	InChI=1S/C9H11Cl3NO2PS/c1-3-14-16(17,13-2)15-9-5-7(11)6(10)4-8(9)12/h4-5H,3H2,1
<b>InchiKey:</b>	WPOYPCBQAYFXJP-UHFFFAOYSA-N
<b>Formula:</b>	C9H11Cl3NO2PS
<b>SMILES:</b>	CCOP(=S)(NC)Oc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	334.59
<b>CAS:</b>	2591-71-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	4.506		Crippen Method
mcvol	209.160	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=C2591711&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2591711&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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