

# O-methyl,o-(2,4,5,-trichlorophenyl)-tert-butyl phosphoramidothioate

<b>Inchi:</b>	InChI=1S/C11H15Cl3NO2PS/c1-11(2,3)15-18(19,16-4)17-10-6-8(13)7(12)5-9(10)14/h5-6
<b>InchiKey:</b>	XPJFSVYYAVAZME-UHFFFAOYSA-N
<b>Formula:</b>	C11H15Cl3NO2PS
<b>SMILES:</b>	COP(=S)(NC(C)(C)C)Oc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	362.64
<b>CAS:</b>	16805-76-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	5.285		Crippen Method
mcvol	237.340	ml/mol	McGowan Method

## Sources

<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>
<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=C16805768&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16805768&amp;Units=SI</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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