

# Iodofenphos

<b>Other names:</b>	(2,5-dichloro-4-iodophenoxy)-dimethoxy-sulfanylidene phosphorane Alfacron C 9491 CIBA C 9491 Ciba 9491 Ciba-geigy C-9491 Compound C-9491 ENT 27408 Elocril Iodfenphos Iodofenfos Iodofenophos Iodophos Jodfenphos Monocron 9491 NSC 190998 Nuvanol N O,O-Dimethyl O-(2,5-dichloro-4-iodophenyl) phosphorothioate O,O-Dimethyl-O-(2,5-dichlor-4-jodphenyl)-monothiophosphat O,O-Dimethyl-O-(2,5-dichlor-4-jodphenyl)-thionophosphat O,O-Dimethyl-O-2,5-dichloro-4-iodophenyl thiophosphate O-(2,5-Dichloro-4-iodophenyl) O,O-dimethyl phosphorothioate OMS 1211 Phosphorothioic acid, O-(2,5-dichloro-4-iodophenyl) O,O-dimethyl ester Trix
<b>Inchi:</b>	InChI=1S/C8H8Cl2IO3PS/c1-12-15(16,13-2)14-8-4-5(9)7(11)3-6(8)10/h3-4H,1-2H3
<b>InchiKey:</b>	LFVLUOAHQIVABZ-UHFFFAOYSA-N
<b>Formula:</b>	C8H8Cl2IO3PS
<b>SMILES:</b>	<chem>COP(=S)(OC)Oc1cc(Cl)c(I)cc1Cl</chem>
<b>Mol. weight [g/mol]:</b>	413.00
<b>CAS:</b>	18181-70-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Aqueous Solubility Prediction Method

log10ws	-6.62		Estimated Solubility Method
logp	4.494		Crippen Method
mcvol	204.540	ml/mol	McGowan Method
rinsol	2150.00		NIST Webbook
rinsol	2150.00		NIST Webbook
tf	345.65	K	Aqueous Solubility Prediction Method

## Sources

<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</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=C18181709&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18181709&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>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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
<b>rinsol:</b>	Non-polar retention indices
<b>tf:</b>	Normal melting (fusion) point

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