

# 2-Furoic acid, 2,3,4,6-tetrachlorophenyl ester

<b>Inchi:</b>	InChI=1S/C11H4Cl4O3/c12-5-4-6(13)10(9(15)8(5)14)18-11(16)7-2-1-3-17-7/h1-4H
<b>InchiKey:</b>	KFKLRDYTWBUVEZ-UHFFFAOYSA-N
<b>Formula:</b>	C11H4Cl4O3
<b>SMILES:</b>	O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1ccco1
<b>Mol. weight [g/mol]:</b>	325.96

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.03		Crippen Method
logp	5.112		Crippen Method
mcvol	184.900	ml/mol	McGowan Method
rinsol	2182.00		NIST Webbook

## Sources

<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=U355176&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355176&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>

## 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

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