

# 3-(2,6-Dichlorophenyl)-5-methyl isoxazole-4-carbonyl chloride

<b>Other names:</b>	Dcimc chloride 4-Isoxazolecarbonyl chloride, 3-(2,6-dichlorophenyl)-5-methyl- 3-(2,6-Dichlorophenyl)-5-methylisoxazole-4-carboxylic acid chloride
<b>Inchi:</b>	InChI=1S/C11H6Cl3NO2/c1-5-8(11(14)16)10(15-17-5)9-6(12)3-2-4-7(9)13/h2-4H,1H3
<b>InchiKey:</b>	IZQGELJKDARDMZ-UHFFFAOYSA-N
<b>Formula:</b>	C11H6Cl3NO2
<b>SMILES:</b>	<chem>Cc1onc(-c2c(Cl)cccc2Cl)c1C(=O)Cl</chem>
<b>Mol. weight [g/mol]:</b>	290.53
<b>CAS:</b>	4462-55-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.31		Crippen Method
logp	4.336		Crippen Method
mcvol	176.770	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4462559&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4462559&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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