

# 4,5-Dichloro-2-methyl-3(2H)-isothiazolone

<b>Other names:</b>	4,5-Dichloro-2-methyl-4-isothiazolin-3-one
<b>Inchi:</b>	InChI=1S/C4H3Cl2NOS/c1-7-4(8)2(5)3(6)9-7/h1H3
<b>InchiKey:</b>	CVZDIUZSWUDGOP-UHFFFAOYSA-N
<b>Formula:</b>	C4H3Cl2NOS
<b>SMILES:</b>	Cn1sc(Cl)c(Cl)c1=O
<b>Mol. weight [g/mol]:</b>	184.04
<b>CAS:</b>	26542-23-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	1.754		Crippen Method
mcvol	104.440	ml/mol	McGowan Method
rinpol	1367.00		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=C26542234&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26542234&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>rinpol:</b>	Non-polar retention indices

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