

# 7-Chloro-s-triazolopyrimidine-5(1H)-one

<b>Inchi:</b>	InChI=1S/C5H3ClN4O/c6-3-1-4(11)10-5(9-3)7-2-8-10/h1-2H,(H,7,8,9)
<b>InchiKey:</b>	OIMZPIMUQKSKGZ-UHFFFAOYSA-N
<b>Formula:</b>	C5H3ClN4O
<b>SMILES:</b>	O=c1cc(Cl)nc2nc[nH]n12
<b>Mol. weight [g/mol]:</b>	170.56

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	-0.411		Crippen Method
mcvol	100.420	ml/mol	McGowan Method
rmpol	1669.00		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=R642130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R642130&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>rmpol:</b>	Non-polar retention indices

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