

# Pyrimidine, 5-allyl-4,6-dichloro-

<b>Inchi:</b>	InChI=1S/C7H6Cl2N2/c1-2-3-5-6(8)10-4-11-7(5)9/h2,4H,1,3H2
<b>InchiKey:</b>	PDLIUMXRLQCZRG-UHFFFAOYSA-N
<b>Formula:</b>	C7H6Cl2N2
<b>SMILES:</b>	C=CCc1c(Cl)ncnc1Cl
<b>Mol. weight [g/mol]:</b>	189.04
<b>CAS:</b>	16019-31-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.512		Crippen Method
mcvol	125.870	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16019311&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16019311&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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