

# Pyrimidine, 4-amino-2,6-dichloro-5-nitro-

<b>Inchi:</b>	InChI=1S/C4H2Cl2N4O2/c5-2-1(10(11)12)3(7)9-4(6)8-2/h(H2,7,8,9)
<b>InchiKey:</b>	HTUHWQWBOTDDW-UHFFFAOYSA-N
<b>Formula:</b>	C4H2Cl2N4O2
<b>SMILES:</b>	<chem>Nc1nc(Cl)nc(Cl)c1[N+](=O)[O-]</chem>
<b>Mol. weight [g/mol]:</b>	208.99
<b>CAS:</b>	31221-68-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	1.274		Crippen Method
mcvol	115.300	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C31221688&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31221688&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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