

# 2,4-Pyrimidinediamine, 6-chloro-5-nitro-

<b>Inchi:</b>	InChI=1S/C4H4ClN5O2/c5-2-1(10(11)12)3(6)9-4(7)8-2/h(H4,6,7,8,9)
<b>InchiKey:</b>	PQRPNYCCQLFXNK-UHFFFAOYSA-N
<b>Formula:</b>	C4H4ClN5O2
<b>SMILES:</b>	<chem>Nc1nc(N)c([N+](=O)[O-])c(Cl)n1</chem>
<b>Mol. weight [g/mol]:</b>	189.56
<b>CAS:</b>	6036-64-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	0.203		Crippen Method
mcvol	113.040	ml/mol	McGowan Method

## 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=C6036642&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6036642&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

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