

# 5-Chloro-2-nitroaniline

<b>Other names:</b>	Benzenamine, 5-chloro-2-nitro- Aniline, 5-chloro-2-nitro- 2-Nitro-5-chloroaniline 3-Chloro-6-nitroaniline 5-Chloro-2-nitrobenzeneamine
<b>Inchi:</b>	InChI=1S/C6H5ClN2O2/c7-4-1-2-6(9(10)11)5(8)3-4/h1-3H,8H2
<b>InchiKey:</b>	ZCWXYZBQDNFULS-UHFFFAOYSA-N
<b>Formula:</b>	C6H5ClN2O2
<b>SMILES:</b>	<chem>Nc1cc(Cl)ccc1[N+](=O)[O-]</chem>
<b>Mol. weight [g/mol]:</b>	172.57
<b>CAS:</b>	1635-61-6

## Physical Properties

Property code	Value	Unit	Source
gf	182.86	kJ/mol	Joback Method
hf	53.71	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	64.17	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.830		Crippen Method
mcvol	111.280	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	635.12	K	Joback Method
tc	902.71	K	Joback Method
tf	465.63	K	Joback Method
vc	0.423	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.95	J/mol×K	635.12	Joback Method
cpg	252.54	J/mol×K	679.72	Joback Method
cpg	260.38	J/mol×K	724.32	Joback Method
cpg	267.52	J/mol×K	768.91	Joback Method

cpg	273.99	J/mol×K	813.51	Joback Method
cpg	279.84	J/mol×K	858.11	Joback Method
cpg	285.10	J/mol×K	902.71	Joback 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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=C1635616&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1635616&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>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<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>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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