

# Benzenamine, 2-chloro-5-nitro-

Other names:	2-Chloro-5-nitroaniline 3-Nitro-6-chloroaniline 6-Chloro-3-nitroaniline Aniline, 2-chloro-5-nitro-
Inchi:	InChI=1S/C6H5C1N2O2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H,8H2
InchiKey:	KWIXNFOTNVKIGM-UHFFFAOYSA-N
Formula:	C6H5C1N2O2
SMILES:	Nc1cc([N+](=O)[O-])ccc1Cl
Mol. weight [g/mol]:	172.57
CAS:	6283-25-6

## 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
hsub	101.00 ± 1.60	kJ/mol	NIST Webbook
hsub	100.30 ± 2.20	kJ/mol	NIST Webbook
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
tt	393.39	K	Solubility Measurement and Thermodynamic Model Correlation and Evaluation of 2-Chloro-5-nitroaniline in 12 Pure Solvents
vc	0.423	m3/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
hsubt	99.30 ± 1.60	kJ/mol	333.00	NIST Webbook

## Sources

<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=C6283256&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6283256&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>Solubility Measurement and Thermodynamic Model Correlation and Evaluation of 2-Chloro-5-nitroaniline in 12 Pure Solvents:</b>	<a href="https://www.doi.org/10.1021/acs.jced.8b00931">https://www.doi.org/10.1021/acs.jced.8b00931</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>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</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>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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