

# 5-Chloro-3-nitro-o-phenylene diamine

<b>Inchi:</b>	InChI=1S/C6H6ClN3O2/c7-3-1-4(8)6(9)5(2-3)10(11)12/h1-2H,8-9H2
<b>InchiKey:</b>	PIPKLZRJGNJMBY-UHFFFAOYSA-N
<b>Formula:</b>	C6H6ClN3O2
<b>SMILES:</b>	<chem>Nc1cc(Cl)cc([N+](=O)[O-])c1N</chem>
<b>Mol. weight [g/mol]:</b>	187.58
<b>CAS:</b>	42389-30-0

## Physical Properties

Property code	Value	Unit	Source
gf	239.68	kJ/mol	Joback Method
hf	76.03	kJ/mol	Joback Method
hfus	30.12	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.413		Crippen Method
mcvol	121.260	ml/mol	McGowan Method
pc	4966.33	kPa	Joback Method
tb	712.63	K	Joback Method
tc	985.51	K	Joback Method
tf	561.41	K	Joback Method
vc	0.453	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.87	J/molxK	712.63	Joback Method
cpg	295.99	J/molxK	758.11	Joback Method
cpg	303.38	J/molxK	803.59	Joback Method
cpg	310.06	J/molxK	849.07	Joback Method
cpg	316.08	J/molxK	894.55	Joback Method
cpg	321.47	J/molxK	940.03	Joback Method
cpg	326.26	J/molxK	985.51	Joback Method

# Sources

<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=C42389300&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42389300&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>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>vc:</b>	Critical Volume

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