

# Phenol, 5-chloro-2-nitro-

<b>Other names:</b>	6-Nitro-3-chlorophenol 5-Chloro-2-nitrophenol
<b>Inchi:</b>	InChI=1S/C6H4ClNO3/c7-4-1-2-5(8(10)11)6(9)3-4/h1-3,9H
<b>InchiKey:</b>	MZDBQSFPAMTTIS-UHFFFAOYSA-N
<b>Formula:</b>	C6H4ClNO3
<b>SMILES:</b>	O=[N+]([O-])c1ccc(Cl)cc1O
<b>Mol. weight [g/mol]:</b>	173.55
<b>CAS:</b>	611-07-4

## Physical Properties

Property code	Value	Unit	Source
gf	-28.58	kJ/mol	Joback Method
hf	-145.92	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hvap	65.88	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.954		Crippen Method
mvol	107.170	ml/mol	McGowan Method
pc	5454.60	kPa	Joback Method
tb	638.23	K	Joback Method
tc	907.39	K	Joback Method
tf	312.00 ± 2.50	K	NIST Webbook
vc	0.360	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.17	J/mol×K	638.23	Joback Method
cpg	243.62	J/mol×K	683.09	Joback Method
cpg	250.40	J/mol×K	727.95	Joback Method
cpg	256.64	J/mol×K	772.81	Joback Method
cpg	262.46	J/mol×K	817.67	Joback Method
cpg	267.97	J/mol×K	862.53	Joback Method
cpg	273.30	J/mol×K	907.39	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=C611074&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C611074&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>hvp:</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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