

# 4-Amino-3-nitrophenol

<b>Other names:</b>	Phenol, 4-amino-3-nitro-
<b>Inchi:</b>	InChI=1S/C6H6N2O3/c7-5-2-1-4(9)3-6(5)8(10)11/h1-3,9H,7H2
<b>InchiKey:</b>	IQXUIDYRTHQTET-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N2O3
<b>SMILES:</b>	<chem>Nc1ccc(O)cc1[N+](=O)[O-]</chem>
<b>Mol. weight [g/mol]:</b>	154.12
<b>CAS:</b>	610-81-1

## Physical Properties

Property code	Value	Unit	Source
gf	49.80	kJ/mol	Joback Method
hf	-96.39	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	72.13	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	0.883		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
pc	6298.82	kPa	Joback Method
tb	673.33	K	Joback Method
tc	945.05	K	Joback Method
tf	534.91	K	Joback Method
vc	0.341	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.94	J/mol×K	673.33	Joback Method
cpg	271.10	J/mol×K	718.62	Joback Method
cpg	278.60	J/mol×K	763.90	Joback Method
cpg	285.57	J/mol×K	809.19	Joback Method
cpg	292.13	J/mol×K	854.48	Joback Method
cpg	298.41	J/mol×K	899.77	Joback Method
cpg	304.53	J/mol×K	945.05	Joback Method

# 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=C610811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C610811&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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