

# N-nitroaniline

<b>Inchi:</b>	InChI=1S/C6H6N2O2/c9-8(10)7-6-4-2-1-3-5-6/h1-5,7H
<b>InchiKey:</b>	VBEGHXKAFSLLGE-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N2O2
<b>SMILES:</b>	O=[N+](O-)Nc1ccccc1
<b>Mol. weight [g/mol]:</b>	138.12
<b>CAS:</b>	645-55-6

## Physical Properties

Property code	Value	Unit	Source
gf	236.99	kJ/mol	Joback Method
hf	112.07	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	54.25	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.290		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
tb	565.37	K	Joback Method
tc	817.61	K	Joback Method
tf	319.15 ± 2.00	K	NIST Webbook
vc	0.381	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.54	J/mol×K	565.37	Joback Method
cpg	231.04	J/mol×K	607.41	Joback Method
cpg	240.66	J/mol×K	649.45	Joback Method
cpg	249.45	J/mol×K	691.49	Joback Method
cpg	257.46	J/mol×K	733.53	Joback Method
cpg	264.74	J/mol×K	775.57	Joback Method
cpg	271.35	J/mol×K	817.61	Joback Method

# Sources

<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>
<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=C645556&amp;Units=SI&amp;Mask=3FFF">http://webbook.nist.gov/cgi/cbook.cgi?ID=C645556&amp;Units=SI&amp;Mask=3FFF</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>mccvol:</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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