

# Benzenamine, N-methyl-4-nitro-

<b>Other names:</b>	4-Nitro-N-methylaniline Aniline, N-methyl-p-nitro- N-(4-Nitrophenyl)-N-methylamine N-Methyl-4-nitroaniline N-Methyl-p-nitraniline N-Methyl-p-nitroaniline N-Monomethyl-p-nitroaniline NSC 5390 p-(Methylamino)nitrobenzene p-Nitro-N-methylaniline
<b>Inchi:</b>	InChI=1S/C7H8N2O2/c1-8-6-2-4-7(5-3-6)9(10)11/h2-5,8H,1H3
<b>InchiKey:</b>	XIFJZJPMHNUGRA-UHFFFAOYSA-N
<b>Formula:</b>	C7H8N2O2
<b>SMILES:</b>	CNc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	152.15
<b>CAS:</b>	100-15-2

## Physical Properties

Property code	Value	Unit	Source
affp	891.60	kJ/mol	NIST Webbook
basg	865.10	kJ/mol	NIST Webbook
chs	-3867.00	kJ/mol	NIST Webbook
gf	235.78	kJ/mol	Joback Method
hf	79.96	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	57.14	kJ/mol	Joback Method
ie	8.17	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	1.636		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
rinpol	1707.00		NIST Webbook
tb	593.23	K	Joback Method
tc	841.00	K	Joback Method
tf	403.86	K	Joback Method
vc	0.436	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.79	J/mol×K	593.23	Joback Method
cpg	275.04	J/mol×K	634.53	Joback Method
cpg	285.42	J/mol×K	675.82	Joback Method
cpg	294.99	J/mol×K	717.12	Joback Method
cpg	303.78	J/mol×K	758.41	Joback Method
cpg	311.84	J/mol×K	799.71	Joback Method
cpg	319.22	J/mol×K	841.00	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.20082e+01
Coeff. B	-3.55065e+03
Coeff. C	-8.72810e+01
Temperature range (K), min.	390.22
Temperature range (K), max.	617.49

## Sources

<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>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=C100152&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C100152&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

# Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chs:</b>	Standard solid enthalpy of combustion
<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>ie:</b>	Ionization energy
<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>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/63-533-0/Benzenamine-N-methyl-4-nitro.pdf>

Generated by Cheméo on 2024-04-19 22:18:47.843978932 +0000 UTC m=+15854376.764556243.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.