

# 1,4-Benzenediamine, 2-nitro-

<b>Other names:</b>	1,4-Diamino-2-nitrobenzene 2,5-Diaminonitrobenzene 2-N-p-PDA 2-NPPD 2-Nitro-1,4-diaminobenzene 2-Nitro-1,4-phenylenediamine 2-Nitrol-p-phenylenediamine 2-nitro-1,4-benzenediamine 2-nitro-4-aminoaniline 2-nitro-p-phenylenediamine 2-nitro-para-phenylenediamine 2-nitrobenzene-1,4-diamine 2NDB 4-Amino-2-nitroaniline C.I. 76070 C.I. Oxidation Base 22 Durafur Brown Durafur Brown 2R Dye GS Fouramine 2R Fourrine 36 Fourrine Brown 2R NCI-C02222 NSC 5377 Nitro-p-phenylenediamine Oxidation base 22 Ursol Brown RR Zoba Brown RR o-Nitro-p-phenylenediamine p-Phenylenediamine, 2-nitro-
<b>Inchi:</b>	InChI=1S/C6H7N3O2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H,7-8H2
<b>InchiKey:</b>	HVHMNGARPCGGD-UHFFFAOYSA-N
<b>Formula:</b>	C6H7N3O2
<b>SMILES:</b>	Nc1ccc(N)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	153.14
<b>CAS:</b>	5307-14-2

# Physical Properties

Property code	Value	Unit	Source
gf	261.24	kJ/mol	Joback Method
hf	103.24	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	70.42	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.759		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	5351.35	kPa	Joback Method
tb	670.22	K	Joback Method
tc	940.43	K	Joback Method
tf	411.35	K	Solubility of 2-nitro-p-phenylenediamine in nine pure solvents and mixture of (methanol + N-methyl-2-pyrrolidone) from T = (283.15 to 318.15) K: Determination and modelling
vc	0.404	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.57	J/mol×K	670.22	Joback Method
cpg	280.82	J/mol×K	715.26	Joback Method
cpg	289.27	J/mol×K	760.29	Joback Method
cpg	296.95	J/mol×K	805.33	Joback Method
cpg	303.92	J/mol×K	850.36	Joback Method
cpg	310.21	J/mol×K	895.40	Joback Method
cpg	315.86	J/mol×K	940.43	Joback Method

# Sources

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Solubility of  
2-nitro-p-phenylenediamine in nine  
pure solvents and mixture of (methanol  
+ N-methyl-2-pyrrolidone) from T =  
(283.15 to 318.15) K: Determination and  
modelling:**

<https://www.doi.org/10.1016/j.jct.2017.01.006>

<b>Experiment and Application of the Solid-Liquid Phase Equilibrium for Ternary Mixture-p-phenylenediamine + Ethyl Acetate + Isopropanol and McGowan Method:</b>	<a href="https://www.doi.org/10.1021/acs.jced.8b00952">https://www.doi.org/10.1021/acs.jced.8b00952</a>
<b>2-Nitro-p-phenylenediamine + 4-Nitro-p-phenylenediamine + N-Methyl-2-pyrrolidone systems:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Crippen Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5307142&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5307142&amp;Units=SI</a>
	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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