1,4-Benzenediamine, 2-nitro-

Other names:	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-
Inchi:	InChI=1S/C6H7N3O2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H,7-8H2
InchiKey:	HVHNMNGARPCGGD-UHFFFAOYSA-N
Formula:	C6H7N3O2
SMILES:	Nc1ccc(N)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	153.14
CAS:	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	m3/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
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

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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume