4-nitro-1,2-benzenediamine

Other names:	(2-amino-4-nitrophenyl)amine
	1,2-diamino-4-nitrobenzene
	2-amino-4-nitroaniline
	4-nitro-1,2-phenylenediamine
	p-nitro-o-phenylenediamine
Inchi:	InChI=1S/C6H7N3O2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H,7-8H2
InchiKey:	RAUWPNXIALNKQM-UHFFFAOYSA-N
Formula:	C6H7N3O2
SMILES:	Nc1ccc([N+](=O)[O-])cc1N
Mol. weight [g/mol]:	153.14

Physical Properties

Property code	Value	Unit	Source
gf	261.24	kJ/mol	Joback Method
hf	103.24	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Solubility determination and modelling of 4-nitro-1,2-phenylenediamine in eleven organic solvents from T = (283.15 to 318.15) K and thermodynamic properties of solutions
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	472.40	K	Solubility determination and modelling of 4-nitro-1,2-phenylenediamine in eleven organic solvents from T = (283.15 to 318.15) K and thermodynamic properties of solutions
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 determination and modelling of 4-nitro-1,2-phenylenediamine in eleven organic solvents from T = (283.15 to 318.15) K and thermodynamic properties of solutions:	https://www.doi.org/10.1016/j.jct.2016.11.014
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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