Benzenamine, 2-chloro-4-nitro-

Other names:	Aniline, 2-chloro-4-nitro-
	o-Chloro-p-nitroaniline
	OCPNA
	1-Amino-2-Chloro-4-nitrobenzene
	2-Chloro-4-nitroaniline
	2-Chloro-4-nitrobenzenamine
	4-Nitro-2-chloroaniline
Inchi:	InChI=1S/C6H5ClN2O2/c7-5-3-4(9(10)11)1-2-6(5)8/h1-3H,8H2
InchiKey:	LOCWBQIWHWIRGN-UHFFFAOYSA-N
Formula:	C6H5ClN2O2
SMILES:	Nc1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]:	172.57
CAS:	121-87-9

Physical Properties

Property code	Value	Unit	Source
gf	182.86	kJ/mol	Joback Method
hf	53.71	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hsub	101.80 ± 1.80	kJ/mol	NIST Webbook
hsub	102.60 ± 1.50	kJ/mol	NIST Webbook
hvap	64.17	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.830		Crippen Method
mcvol	111.280	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	635.12	K	Joback Method
tc	902.71	K	Joback Method
tf	465.63	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	243.95	J/mol×K	635.12	Joback Method
cpg	252.54	J/mol×K	679.72	Joback Method
cpg	260.38	J/mol×K	724.32	Joback Method
cpg	267.52	J/mol×K	768.91	Joback Method
cpg	273.99	J/mol×K	813.51	Joback Method
cpg	279.84	J/mol×K	858.11	Joback Method
cpg	285.10	J/mol×K	902.71	Joback Method
hsubt	100.30 ± 1.50	kJ/mol	343.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C121879&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
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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