

# 5-Chloro-4-fluoro-2-nitroaniline

## InChI:

InChI=1S/C6H4ClFN2O2/c7-3-1-5(9)6(10(11)12)2-4(3)8/h1-2H,9H2

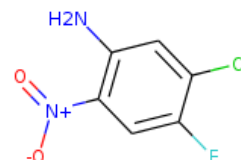
**InChI Key:** VRJKEIWZSOHDOH-UHFFFAOYSA-N

**Formula:** C6H4ClFN2O2

**SMILES:** Nc1cc(Cl)c(F)cc1[N+](=O)[O-]

**Molecular Weight:** 190.56

**CAS:** 104222-34-6



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-21.58	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-153.87	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	28.01	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	64.01	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.97		Crippen Method
$P_c$	4322.57	kPa	Joback Method
$T_{\text{boil}}$	639.37	K	Joback Method
$T_c$	894.41	K	Joback Method
$T_{\text{fus}}$	478.74	K	Joback Method
$V_c$	0.44	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	250.35	J/mol×K	639.37	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:**

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H4ClFN2O2/c7-3-1-5\(9\)6\(10\(11\)12\)2-4\(3\)8/h1-2H,9H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H4ClFN2O2/c7-3-1-5(9)6(10(11)12)2-4(3)8/h1-2H,9H2)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$C_{p, gas}$ : Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{oct/wat}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{boil}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{fus}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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