

# 1-Nitro-4-propylbenzene

**Other names:** 4-Nitro-n-propylbenzene; Benzene, 1-nitro-4-propyl-; p-Nitropropylbenzene; p-Propylnitrobenzene.

**InChI:**

InChI=1S/C9H11NO2/c1-2-3-8-4-6-9(7-5-8)10(11)12/h4-7H,2-3H2,1H3

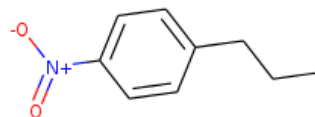
**InChI Key:** SXQBFCVVZIYXHV-UHFFFAOYSA-N

**Formula:** C9H11NO2

**SMILES:** CCCc1ccc([N+](=O)[O-])cc1

**Molecular Weight:** 165.19

**CAS:** 10342-59-3



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	163.23	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-14.79	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	24.08	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	55.16	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.55		Crippen Method
$P_c$	3250.43	kPa	Joback Method
$T_{\text{boil}}$	588.82	K	Joback Method
$T_c$	828.33	K	Joback Method
$T_{\text{fus}}$	373.74	K	Joback Method
$V_c$	0.51	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	310.78	J/mol×K	588.82	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/C9H11NO2/c1-2-3-8-4-6-9\(7-5-8\)10\(11\)12/h4-7H,2-3H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H11NO2/c1-2-3-8-4-6-9(7-5-8)10(11)12/h4-7H,2-3H2,1H3)

**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).

$logP_{oct/wat}$ : 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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