

# P-toluic acid, 4-cyanophenyl ester

**Other names:** p-Toluylic acid, 4-cyanophenyl ester.

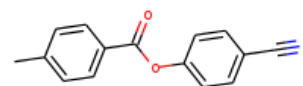
**InChI:** InChI=1S/C15H11NO2/c1-11-2-6-13(7-3-11)15(17)18-14-8-4-12(10-16)5-9-14/h2-9H,1H3

**InChI Key:** QIAWNOODTBZTGG-UHFFFAOYSA-N

**Formula:** C15H11NO2

**SMILES:** Cc1ccc(C(=O)Oc2ccc(C#N)cc2)cc1

**Molecular Weight:** 237.25



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	180.24	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	17.27	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	26.20	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	74.49	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.09		Crippen Method
$P_c$	2487.55	kPa	Joback Method
$T_{\text{boil}}$	784.29	K	Joback Method
$T_c$	1033.83	K	Joback Method
$T_{\text{fus}}$	473.84	K	Joback Method
$V_c$	0.71	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	483.85	J/mol×K	784.29	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/C15H11NO2/c1-11-2-6-13\(7-3-11\)15\(17\)18-14-8-4-12\(10-16\)5-9-14/h2-9H,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H11NO2/c1-11-2-6-13(7-3-11)15(17)18-14-8-4-12(10-16)5-9-14/h2-9H,1H3)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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