

# 1-Naphthoic acid, 4-cyanophenyl ester

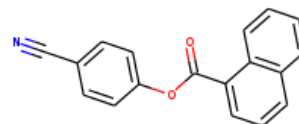
**InChI:** InChI=1S/C18H11NO2/c19-12-13-8-10-15(11-9-13)21-18(20)17-7-3-5-14-4-1-2-6-16(14)17/h1-11H

**InChI Key:** XJZYDLZARKPZFG-UHFFFAOYSA-N

**Formula:** C18H11NO2

**SMILES:** N#Cc1ccc(OC(=O)c2cccc3ccccc32)cc1

**Molecular Weight:** 273.29



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	312.15	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	146.42	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	30.99	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	82.81	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.93		Crippen Method
$P_c$	2384.19	kPa	Joback Method
$T_{\text{boil}}$	871.91	K	Joback Method
$T_c$	1132.38	K	Joback Method
$T_{\text{fus}}$	540.35	K	Joback Method
$V_c$	0.80	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	568.09	J/mol×K	871.91	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/C18H11NO2/c19-12-13-8-10-15\(11-9-13\)21-18\(20\)17-7-3-5-14-4-1-2-6-16\(14\)17/h1-11H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H11NO2/c19-12-13-8-10-15(11-9-13)21-18(20)17-7-3-5-14-4-1-2-6-16(14)17/h1-11H)

**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).

Latest version available from:

<https://www.cheméo.com/cid/60-052-7/1-Naphthoic%20acid%2C%204-cyanophenyl%20ester>

Generated by Cheméo on Sat, 18 Sep 2021 09:45:25 +0000.

**Cheméo** (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.