

O-cyanobenzoic acid

Other names: 2-Cyanobenzoic acid; Benzoic acid, 2-cyano-

InChI: InChI=1S/C8H5NO2/c9-5-6-3-1-2-4-7(6)8(10)11/h1-4H,(H,10,11)

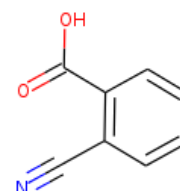
InChI Key: DTNSDCJFTHMDAK-UHFFFAOYSA-N

Formula: C8H5NO2

SMILES: N#Cc1ccccc1C(=O)O

Molecular Weight: 147.13

CAS: 3839-22-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-13.30	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-83.32	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	17.32	kJ/mol	Joback Method
$\Delta_{\text{sub}} H^\circ$	114.60 ± 1.30	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	70.24	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.26		Crippen Method
P_c	4216.56	kPa	Joback Method
T_{boil}	662.23	K	Joback Method
T_c	883.54	K	Joback Method
T_{fus}	394.60	K	Joback Method
V_c	0.43	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	247.34	J/mol×K	662.23	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H5NO2/c9-5-6-3-1-2-4-7\(6\)8\(10\)11/h1-4H,\(H,10,11\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H5NO2/c9-5-6-3-1-2-4-7(6)8(10)11/h1-4H,(H,10,11))

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).

$\Delta_{sub} H^\circ$: Enthalpy of sublimation 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 (m³/kg-mol).

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