

4-Cyanobenzoic acid, heptyl ester

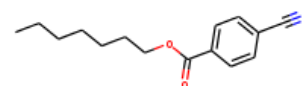
InChI: InChI=1S/C15H19NO2/c1-2-3-4-5-6-11-18-15(17)14-9-7-13(12-16)
8-10-14/h7-10H,2-6,11H2,1H3

InChI Key: QNDZVAFNIKAYET-UHFFFAOYSA-N

Formula: C₁₅H₁₉NO₂

SMILES: CCCCCCOC(=O)c1ccc(C#N)cc1

Molecular Weight: 245.32



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	77.46	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-207.79	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	32.55	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	71.56	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.69		Crippen Method
P_c	1856.31	kPa	Joback Method
T_{boil}	752.63	K	Joback Method
T_c	963.66	K	Joback Method
T_{fus}	434.90	K	Joback Method
V_c	0.82	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	577.27	J/mol×K	752.63	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H19NO2/c1-2-3-4-5-6-11-18-15\(17\)14-9-7-13\(12-16\)8-10-14/h7-10H,2-6,11H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H19NO2/c1-2-3-4-5-6-11-18-15(17)14-9-7-13(12-16)8-10-14/h7-10H,2-6,11H2,1H3)

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 (m³/kg-mol).

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