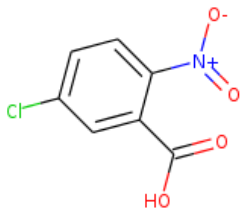
5-Chloro-2-nitrobenzoic acid

Other names: Benzoic acid, 5-chloro-2-nitro-.
InChI:
InChI=1S/C7H4ClNO4/c8-4-1-2-6(9(12)13)5(3-4)7(10)11/h1-3H,(H,10,11)
InChI Key: ZKUYSJHXBFFGPU-UHFFFAOYSA-N
Formula: C7H4ClNO4
SMILES: O=C(O)c1cc(Cl)ccc1[N+](=O)[O-]
Molecular Weight: 201.56
CAS: 2516-95-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-140.91	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-265.53	kJ/mol	Joback Method
$\Delta_{fus} H°$	28.39	kJ/mol	Joback Method
$\Delta_{vap} H°$	79.18	kJ/mol	Joback Method
$logP_{oct/wat}$	1.95		Crippen Method
P_c	4697.74	kPa	Joback Method
T_{boil}	731.52	K	Joback Method
T_c	968.96	K	Joback Method
T_{fus}	504.39	K	Joback Method
V_c	0.48	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	283.94	J/mol×K	731.52	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H4ClNO4/c8-4-1-2-6(9(12)13)5(3-4)7(10)11/h1-3H,(H,10,11)

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).