p-Chlorophenol

Other names: 4-Chlorophenol; 4-Hydroxychlorobenzene; Applied 3-78; NSC 2877; Parachlorophenol; Phenol, p-chloro-; p-Chlorfenol; p-Chlorophenic acid; p-Chlorophenol.

InChI: InChI=1S/C6H5ClO/c7-5-1-3-6(8)4-2-5/h1-4,8H

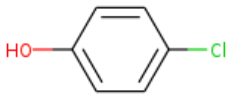
InChI Key: WXNZTHHGJRFXKQ-UHFFFAOYSA-N

Formula: C6H5ClO

SMILES: Oc1ccc(Cl)cc1

Molecular Weight: 128.56

CAS: 106-48-9



Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{liquid}$	-2917.90 ± 8.40	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-2901.60 ± 8.40	kJ/mol	NIST Webbook
$\Delta_f G°$	-54.50	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-123.69	kJ/mol	Joback Method
$\Delta_{fus} H°$	15.32	kJ/mol	Joback Method
$\Delta_{sub} H°$	77.10 ± 0.20	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	64.40 ± 0.30	kJ/mol	NIST Webbook
IE	9.07	eV	NIST Webbook
IE	8.69	eV	NIST Webbook
$logP_{oct/wat}$	2.05		Crippen Method
P_c	5478.85	kPa	Joback Method
T_{boil}	492.90	K	NIST Webbook
T_{boil}	492.90 ± 0.40	K	NIST Webbook
T_c	721.38	K	Joback Method
T_{fus}	316.00 ± 0.20	K	NIST Webbook
V_c	0.28	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	167.36	J/mol×K	481.41	Joback Method
η	0.00	Pa×s	481.41	Joback Method
$\Delta_{fus}H$	14.07	kJ/mol	315.9	NIST Webbook
$\Delta_{fus}H$	14.07	kJ/mol	315.9	NIST Webbook
$\Delta_{fus}H$	14.07	kJ/mol	316.0	NIST Webbook
$\Delta_{sub}H$	60.80	kJ/mol	272.5	NIST Webbook
$\Delta_{sub}H$	54.00 ± 1.00	kJ/mol	297.0	NIST Webbook
$\Delta_{vap}H$	61.90	kJ/mol	334.5	NIST Webbook
$\Delta_{vap}H$	52.80	kJ/mol	408.0	NIST Webbook
$\Delta_{vap}H$	60.60	kJ/mol	433.0	NIST Webbook
$\Delta_{fus}S$	44.51	J/mol×K	316.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H5ClO/c7-5-1-3-6(8)4-2-5/h1-4,8H
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_c\mathbf{H°_{liquid}}$: Standard liquid enthalpy of combustion (kJ/mol).
$\Delta_c\mathbf{H°_{solid}}$: Standard solid enthalpy of combustion (kJ/mol).
$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H}$: Enthalpy of fusion at a given temperature (kJ/mol).
$\Delta_{sub}\mathbf{H°}$: Enthalpy of sublimation at standard conditions (kJ/mol).
$\Delta_{sub}\mathbf{H}$: Enthalpy of sublimation at a given temperature (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H}$: Enthalpy of vaporization at a given temperature (kJ/mol).

IE: Ionization energy (eV).

***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .

P$_c$: Critical Pressure (kPa).

Δ_{fus}**S**: Entropy of fusion at a given temperature (J/mol×K).

T$_{boil}$: Normal Boiling Point Temperature (K).

T$_c$: Critical Temperature (K).

T$_{fus}$: Normal melting (fusion) point (K).

V$_c$: Critical Volume (m^3/kg-mol).