5-Chlorosalicylic acid

Other names: 2-Hydroxy-5-chlorobenzoic acid; 5 CSA; 5-Chloro-2-hydroxybenzoic acid; 5-Chlorosalicylic acid; Salicylic acid, 5-chloro-.

InChI: InChI=1S/C7H5ClO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,(H,10,11)

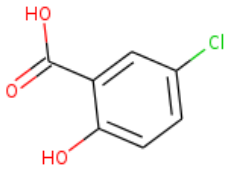
InChI Key: NKBASRXWGAGQDP-UHFFFAOYSA-N

Formula: C7H5ClO3

SMILES: O=C(O)c1cc(Cl)ccc1O

Molecular Weight: 172.57

CAS: 321-14-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-321.45	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-420.61	kJ/mol	Joback Method
$\Delta_{fus} H°$	23.21	kJ/mol	Joback Method
$\Delta_{vap} H°$	74.94	kJ/mol	Joback Method
$logP_{oct/wat}$	1.74		Crippen Method
P_c	5853.95	kPa	Joback Method
T_{boil}	655.32	K	Joback Method
T_c	879.90	K	Joback Method
T_{fus}	459.98	K	Joback Method
V_c	0.36	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	249.69	J/mol×K	655.32	Joback Method
η	0.00	Pa×s	655.32	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H5ClO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,(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).
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).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).