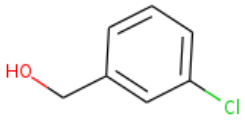
3-Chlorobenzyl alcohol

Other names: Benzenemethanol, 3-chloro-; m-Chlorobenzyl alcohol.
InChI: InChI=1S/C7H7ClO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5H2
InChI Key: ZSRDNPVYGSFUMD-UHFFFAOYSA-N
Formula: C7H7ClO
SMILES: OCc1cccc(Cl)c1
Molecular Weight: 142.58
CAS: 873-63-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-37.91	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-130.72	kJ/mol	Joback Method
$\Delta_{fus} H°$	15.82	kJ/mol	Joback Method
$\Delta_{vap} H°$	55.18	kJ/mol	Joback Method
IE	8.51	eV	NIST Webbook
$logP_{oct/wat}$	1.83		Crippen Method
P_c	4333.96	kPa	Joback Method
T_{boil}	510.20	K	NIST Webbook
T_c	727.48	K	Joback Method
T_{fus}	298.33	K	Joback Method
V_c	0.39	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	204.63	J/mol×K	520.83	Joback Method
η	0.00	Pa×s	520.83	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H7ClO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5H2
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).
IE: Ionization energy (eV).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).