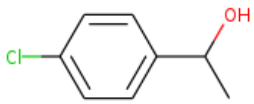
4-Chloro-alpha-methylbenzyl alcohol

Other names: 1-(4-Chlorophenyl)ethanol; 1-(p-Chlorophenyl)ethanol; 1-p-Chlorophenylethyl alcohol; 4-Chloro-alpha-methylbenzyl alcohol; 4-Chlorophenylmethylcarbinol; 4-chloro-«alpha»-methylbenzyl alcohol; Benzyl alcohol, p-chloro-«alpha»-methyl-; p-Chloro-«alpha»-methylbenzyl alcohol; «alpha»-(p-Chlorophenyl)ethanol.



InChI: InChI=1S/C8H9ClO/c1-6(10)7-2-4-8(9)5-3-7/h2-6,10H,1H3

InChI Key: MVOSNPUNXINWAD-UHFFFAOYSA-N

Formula: C8H9ClO

SMILES: CC(O)c1ccc(Cl)cc1

Molecular Weight: 156.61

CAS: 3391-10-4

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-31.93	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-156.64	kJ/mol	Joback Method
$\Delta_{fus} H°$	14.89	kJ/mol	Joback Method
$\Delta_{vap} H°$	57.02	kJ/mol	Joback Method
$log P_{oct/wat}$	2.39		Crippen Method
P_c	3872.29	kPa	Joback Method
T_{boil}	543.27	K	Joback Method
T_c	751.23	K	Joback Method
T_{fus}	294.60	K	Joback Method
V_c	0.44	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	247.37	J/mol×K	543.27	Joback Method
η	0.00	Pa×s	543.27	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H9ClO/c1-6(10)7-2-4-8(9)5-3-7/h2-6,10H,1H3
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).