P-toluic acid, 3-chloro-

Other names: 3-Chloro-4-methylbenzoic acid; 3-Chloro-p-toluic acid; Benzoic acid, 3-chloro-4-methyl-.

InChI: InChI=1S/C8H7ClO2/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4H,1H3,(H,10,11)

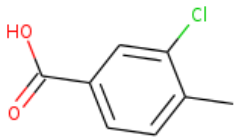
InChI Key: SDKUOEOJAXGCLU-UHFFFAOYSA-N

Formula: C8H7ClO2

SMILES: Cc1ccc(C(=O)O)cc1Cl

Molecular Weight: 170.59

CAS: 5162-82-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-168.04	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-275.41	kJ/mol	Joback Method
$\Delta_{fus} H°$	19.62	kJ/mol	Joback Method
$\Delta_{vap} H°$	64.81	kJ/mol	Joback Method
$logP_{oct/wat}$	2.35		Crippen Method
P_c	4072.51	kPa	Joback Method
T_{boil}	602.56	K	Joback Method
T_c	814.98	K	Joback Method
T_{fus}	372.05	K	Joback Method
V_c	0.45	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	256.09	J/mol×K	602.56	Joback Method
η	0.00	Pa×s	602.56	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H7ClO2/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4H,1H3,(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).