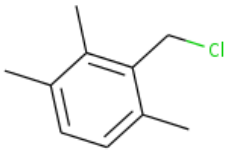
1,2,4-Trimethyl-3-(chloromethyl)benzene

InChI: InChI=1S/C10H13Cl/c1-7-4-5-8(2)10(6-11)9(7)3/h4-5H,6H2,1-3H3
InChI Key: HGFIBEDXILACRG-UHFFFAOYSA-N
Formula: C10H13Cl
SMILES: Cc1ccc(C)c(CCl)c1C
Molecular Weight: 168.66



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	104.91	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-63.35	kJ/mol	Joback Method
$\Delta_{fus} H°$	18.73	kJ/mol	Joback Method
$\Delta_{vap} H°$	46.50	kJ/mol	Joback Method
$logP_{oct/wat}$	3.35		Crippen Method
P_c	2687.42	kPa	Joback Method
T_{boil}	507.25	K	Joback Method
T_c	721.45	K	Joback Method
T_{fus}	296.36	K	Joback Method
V_c	0.54	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	285.86	J/mol×K	507.25	Joback Method
η	0.00	Pa×s	507.25	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H13Cl/c1-7-4-5-8(2)10(6-11)9(7)3/h4-5H,6H2,1-3H3
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).