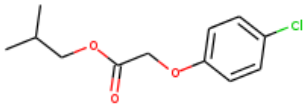
Acetic acid, (4-chlorophenoxy)-, isobutyl ester

InChI: InChI=1S/C12H15ClO3/c1-9(2)7-16-12(14)8-15-11-5-3-10(13)4-6-11/h3-6,9H,7-8H2,1-2H3
InChI Key: KPZQJZLKVMNLLD-UHFFFAOYSA-N
Formula: C12H15ClO3
SMILES: CC(C)COC(=O)COc1ccc(Cl)cc1
Molecular Weight: 242.70



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-200.35	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-463.99	kJ/mol	Joback Method
$\Delta_{fus} H°$	25.14	kJ/mol	Joback Method
$\Delta_{vap} H°$	60.81	kJ/mol	Joback Method
$logP_{oct/wat}$	2.92		Crippen Method
P_c	2370.28	kPa	Joback Method
T_{boil}	641.32	K	Joback Method
T_c	854.00	K	Joback Method
T_{fus}	373.25	K	Joback Method
V_c	0.68	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	447.02	J/mol×K	641.32	Joback Method
η	0.00	Pa×s	641.32	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H15ClO3/c1-9(2)7-16-12(14)8-15-11-5-3-10(13)4-6-11/h3-6,9H,7-8H2,1-2H3
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).