Phenylacetic acid, 4-chloro-, tridecyl ester

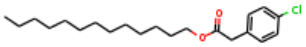
InChI: InChI=1S/C21H33ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-21(23)18-19-13-15-20(22)16-14-19/h13-16H,2-12,17-18H2,1H3

InChI Key: LECJSGBIFXEKSF-UHFFFAOYSA-N

Formula: C21H33ClO2

SMILES: CCCCCCCCCCCCCOC(=O)Cc1ccc(Cl)cc1

Molecular Weight: 352.94



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-17.13	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-512.25	kJ/mol	Joback Method
$\Delta_{fus} H°$	50.78	kJ/mol	Joback Method
$\Delta_{vap} H°$	78.82	kJ/mol	Joback Method
$logP_{oct/wat}$	6.74		Crippen Method
P_c	1181.71	kPa	Joback Method
T_{boil}	825.26	K	Joback Method
T_c	1021.88	K	Joback Method
T_{fus}	467.45	K	Joback Method
V_c	1.18	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	916.32	J/mol×K	825.26	Joback Method
η	0.00	Pa×s	825.26	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H33ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-21(23)18-19-13-15-20(22)16-14-19/h13-16H,2-12,17-18H2,1H3
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).