Phthalic acid, 2,2-dichloroethyl tridecyl ester

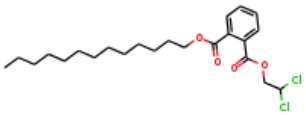
InChI: InChI=1S/C23H34Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-28-22(26)19-15-12-13-16-20(19)23(27)29-18-21(24)25/h12-13,15-16,21H,2-11,14,17-18H2,1H3

InChI Key: UMLKZQZCQZHFGI-UHFFFAOYSA-N

Formula: C23H34Cl2O4

SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(Cl)Cl

Molecular Weight: 445.42



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-248.58	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-819.35	kJ/mol	Joback Method
$\Delta_{fus} H°$	59.42	kJ/mol	Joback Method
$\Delta_{vap} H°$	96.42	kJ/mol	Joback Method
$logP_{oct/wat}$	7.11		Crippen Method
P_c	1051.41	kPa	Joback Method
T_{boil}	984.30	K	Joback Method
T_c	1205.36	K	Joback Method
T_{fus}	577.07	K	Joback Method
V_c	1.36	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1110.16	J/mol×K	984.3	Joback Method
η	0.00	Pa×s	984.3	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H34Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-28-22(26)19-15-12-13-16-20(19)23(27)29-18-21(24)25/h12-13,15-16,21H,2-11,14,17-18H2,1H3
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).