Dimethylmalonic acid, propyl 2,3,5-trichlorophenyl ester

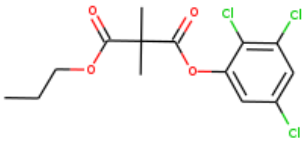
InChI: InChI=1S/C14H15Cl3O4/c1-4-5-20-12(18)14(2,3)13(19)21-10-7-8(15)6-9(16)11(10)17/h6-7H,4-5H2,1-3H3

InChI Key: PEGMVXZLURBLDL-UHFFFAOYSA-N

Formula: C14H15Cl3O4

SMILES: CCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)cc(Cl)c1Cl

Molecular Weight: 353.62



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-350.27	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-675.74	kJ/mol	Joback Method
$\Delta_{fus} H°$	35.64	kJ/mol	Joback Method
$\Delta_{vap} H°$	81.19	kJ/mol	Joback Method
$logP_{oct/wat}$	4.53		Crippen Method
P_c	1930.44	kPa	Joback Method
T_{boil}	822.98	K	Joback Method
T_c	1049.66	K	Joback Method
T_{fus}	548.02	K	Joback Method
V_c	0.90	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	611.60	J/mol×K	822.98	Joback Method
η	0.00	Pa×s	822.98	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H15Cl3O4/c1-4-5-20-12(18)14(2,3)13(19)21-10-7-8(15)6-9(16)11(10)17/h6-7H,4-5H2,1-3H3
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).