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

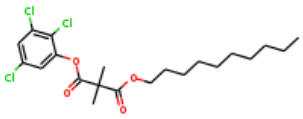
InChI: InChI=1S/C21H29Cl3O4/c1-4-5-6-7-8-9-10-11-12-27-19(25)21(2,3)20(26)28-17-14-15(22)13-16(23)18(17)24/h13-14H,4-12H2,1-3H3

InChI Key: BPYNSAWLBYJABD-UHFFFAOYSA-N

Formula: C21H29Cl3O4

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

Molecular Weight: 451.81



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-291.33	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-820.22	kJ/mol	Joback Method
$\Delta_{fus} H°$	53.77	kJ/mol	Joback Method
$\Delta_{vap} H°$	96.77	kJ/mol	Joback Method
$logP_{oct/wat}$	7.26		Crippen Method
P_c	1150.65	kPa	Joback Method
T_{boil}	983.14	K	Joback Method
T_c	1207.14	K	Joback Method
T_{fus}	626.91	K	Joback Method
V_c	1.29	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1010.50	J/mol×K	983.14	Joback Method
η	0.00	Pa×s	983.14	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H29Cl3O4/c1-4-5-6-7-8-9-10-11-12-27-19(25)21(2,3)20(26)28-17-14-15(22)13-16(23)18(17)24/h13-14H,4-12H2,1-3H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).