Dimethylmalonic acid, heptyl 3-phenylpropyl ester

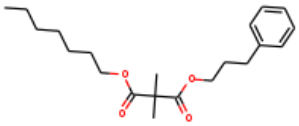
InChI: InChI=1S/C21H32O4/c1-4-5-6-7-11-16-24-19(22)21(2,3)20(23)25-17-12-15-18-13-9-8-10-14-18/h8-10,13-14H,4-7,11-12,15-17H2,1-3H3

InChI Key: JPBMFFPSKJVVCN-UHFFFAOYSA-N

Formula: C21H32O4

SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)OCCCc1ccccc1

Molecular Weight: 348.48



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-226.65	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-738.59	kJ/mol	Joback Method
$\Delta_{fus} H°$	42.35	kJ/mol	Joback Method
$\Delta_{vap} H°$	81.63	kJ/mol	Joback Method
$logP_{oct/wat}$	4.70		Crippen Method
P_c	1282.83	kPa	Joback Method
T_{boil}	855.91	K	Joback Method
T_c	1060.47	K	Joback Method
T_{fus}	499.59	K	Joback Method
V_c	1.14	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	938.54	J/mol×K	855.91	Joback Method
η	0.00	Pa×s	855.91	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H32O4/c1-4-5-6-7-11-16-24-19(22)21(2,3)20(23)25-17-12-15-18-13-9-8-10-14-18/h8-10,13-14H,4-7,11-12,15-17H2,1-3H3
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).