Dimethylmalonic acid, ethyl 3-nitrophenyl ester

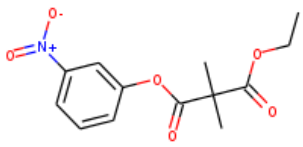
InChI: InChI=1S/C13H15NO6/c1-4-19-11(15)13(2,3)12(16)20-10-7-5-6-9(8-10)14(17)18/h5-8H,4H2,1-3H3

InChI Key: HKGFQZNVWYAOCJ-UHFFFAOYSA-N

Formula: C13H15NO6

SMILES: CCOC(=O)C(C)(C)C(=O)Oc1cccc([N+](=O)[O-])c1

Molecular Weight: 281.26



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-268.09	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-595.70	kJ/mol	Joback Method
$\Delta_{fus} H°$	32.60	kJ/mol	Joback Method
$\Delta_{vap} H°$	81.08	kJ/mol	Joback Method
$logP_{oct/wat}$	2.09		Crippen Method
P_c	2433.84	kPa	Joback Method
T_{boil}	829.69	K	Joback Method
T_c	1068.02	K	Joback Method
T_{fus}	565.56	K	Joback Method
V_c	0.77	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	589.03	J/mol×K	829.69	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H15NO6/c1-4-19-11(15)13(2,3)12(16)20-10-7-5-6-9(8-10)14(17)18/h5-8H,4H2,1-3H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: 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).