Diethylmalonic acid, di(2-octyl) ester

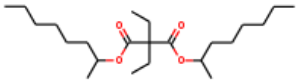
InChI: InChI=1S/C23H44O4/c1-7-11-13-15-17-19(5)26-21(24)23(9-3,10-4)22(25)27-20(6)18-16-14-12-8-2/h19-20H,7-18H2,1-6H3

InChI Key: SSWHDFOWSMCOKF-UHFFFAOYSA-N

Formula: C23H44O4

SMILES: CCCCCCC(C)OC(=O)C(CC)(CC)C(=O)OC(C)CCCCCC

Molecular Weight: 384.59



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-327.10	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1026.96	kJ/mol	Joback Method
$\Delta_{fus} H°$	46.44	kJ/mol	Joback Method
$\Delta_{vap} H°$	83.03	kJ/mol	Joback Method
$logP_{oct/wat}$	6.60		Crippen Method
P_c	918.83	kPa	Joback Method
T_{boil}	874.11	K	Joback Method
T_c	1070.79	K	Joback Method
T_{fus}	465.71	K	Joback Method
V_c	1.35	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1155.68	J/mol×K	874.11	Joback Method
η	0.00	Pa×s	874.11	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H44O4/c1-7-11-13-15-17-19(5)26-21(24)23(9-3,10-4)22(25)27-20(6)18-16-14-12-8-2/h19-20H,7-18H2,1-6H3
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).