Diethylmalonic acid, dodecyl 5-methoxy-3-methylpentyl ester

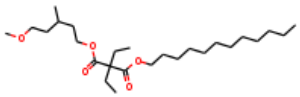
InChI: InChI=1S/C26H50O5/c1-6-9-10-11-12-13-14-15-16-17-20-30-24(27)26(7-2,8-3)25(28)31-22-19-23(4)18-21-29-5/h23H,6-22H2,1-5H3

InChI Key: BHRYEPQCALICHN-UHFFFAOYSA-N

Formula: C26H50O5

SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCOC

Molecular Weight: 442.67



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-404.40	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1215.82	kJ/mol	Joback Method
$\Delta_{fus} H°$	58.92	kJ/mol	Joback Method
$\Delta_{vap} H°$	92.51	kJ/mol	Joback Method
$logP_{oct/wat}$	6.86		Crippen Method
P_c	766.49	kPa	Joback Method
T_{boil}	965.61	K	Joback Method
T_c	1187.20	K	Joback Method
T_{fus}	536.75	K	Joback Method
V_c	1.54	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1377.22	J/mol×K	965.61	Joback Method
η	0.00	Pa×s	965.61	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H50O5/c1-6-9-10-11-12-13-14-15-16-17-20-30-24(27)26(7-2,8-3)25(28)31-22-19-23(4)18-21-29-5/h23H,6-22H2,1-5H3
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).