Succinic acid, dodec-2-enyl 3-methylbutyl ester

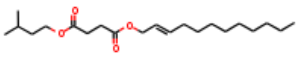
InChI: InChI=1S/C21H38O4/c1-4-5-6-7-8-9-10-11-12-13-17-24-20(22)14-15-21(23)25-18-16-19(2)3/h12-13,19H,4-11,14-18H2,1-3H3/b13-12+

InChI Key: QUPIVGPMNXQHKB-OUKQBFOZSA-N

Formula: C21H38O4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)OCCC(C)C

Molecular Weight: 354.52



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-264.12	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-854.43	kJ/mol	Joback Method
$\Delta_{fus} H°$	52.40	kJ/mol	Joback Method
$\Delta_{vap} H°$	80.22	kJ/mol	Joback Method
$logP_{oct/wat}$	5.60		Crippen Method
P_c	1052.77	kPa	Joback Method
T_{boil}	836.18	K	Joback Method
T_c	1026.01	K	Joback Method
T_{fus}	450.67	K	Joback Method
V_c	1.23	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1004.95	J/mol×K	836.18	Joback Method
η	0.00	Pa×s	836.18	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H38O4/c1-4-5-6-7-8-9-10-11-12-13-17-24-20(22)14-15-21(23)25-18-16-19(2)3/h12-13,19H,4-11,14-18H2,1-3H3/b13-12+
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).