Sebacic acid, 2,4-dimethylpent-3-yl pentadecyl ester

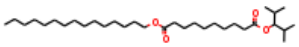
InChI: InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-32(33)25-22-19-16-17-20-23-26-31(34)36-32(28(2)3)29(4)5/h28-29,32H,6-27H2,1-5H3

InChI Key: IQDRZKWTALQNIE-UHFFFAOYSA-N

Formula: C32H62O4

SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C

Molecular Weight: 510.83



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-256.60	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1209.25	kJ/mol	Joback Method
$\Delta_{fus} H°$	73.64	kJ/mol	Joback Method
$\Delta_{vap} H°$	103.97	kJ/mol	Joback Method
$logP_{oct/wat}$	9.97		Crippen Method
P_c	573.98	kPa	Joback Method
T_{boil}	1082.82	K	Joback Method
T_c	1370.02	K	Joback Method
T_{fus}	549.72	K	Joback Method
V_c	1.86	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1737.08	J/mol×K	1082.82	Joback Method
η	0.00	Pa×s	1082.82	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30(33)25-22-19-16-17-20-23-26-31(34)36-32(28(2)3)29(4)5/h28-29,32H,6-27H2,1-5H3
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).