Sebacic acid, 2-hexyl pentadecyl ester

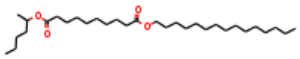
InChI: InChI=1S/C31H60O4/c1-4-6-8-9-10-11-12-13-14-15-18-21-24-28-34-30(32)26-22-19-16-17-20-23-27-31(33)35-29(3)25-7-5-2/h29H,4-28H2,1-3H3

InChI Key: RNWKLGRMLBVKEQ-UHFFFAOYSA-N

Formula: C31H60O4

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

Molecular Weight: 496.81



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-260.14	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1178.05	kJ/mol	Joback Method
$\Delta_{fus} H°$	78.10	kJ/mol	Joback Method
$\Delta_{vap} H°$	102.52	kJ/mol	Joback Method
$logP_{oct/wat}$	9.863		Crippen Method
P_c	596.63	kPa	Joback Method
T_{boil}	1060.82	K	Joback Method
T_c	1339.85	K	Joback Method
T_{fus}	568.45	K	Joback Method
V_c	1.813	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1671.04	J/mol×K	1060.82	Joback Method
η	0.0000088	Pa×s	1060.82	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C31H60O4/c1-4-6-8-9-10-11-12-13-14-15-18-21-24-28-34-30(32)26-22-19-16-17-20-23-27-31(33)35-29(3)25-7-5-2/h29H,4-28H2,1-3H3
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).