Pimelic acid, phenethyl undecyl ester

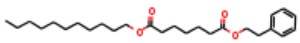
InChI: InChI=1S/C26H42O4/c1-2-3-4-5-6-7-8-9-16-22-29-25(27)19-14-11-15-20-26(28)30-23-21-24-17-12-10-13-18-24/h10,12-13,17-18H,2-9,11,14-16,19-23H2,1H3

InChI Key: LIJBHUXCFIKBEC-UHFFFAOYSA-N

Formula: C26H42O4

SMILES: CCCCCCCCCCCOC(=O)CCCCCC(=O)OCCc1ccccc1

Molecular Weight: 418.61



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-187.39	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-833.04	kJ/mol	Joback Method
$\Delta_{fus} H°$	62.71	kJ/mol	Joback Method
$\Delta_{vap} H°$	94.06	kJ/mol	Joback Method
$logP_{oct/wat}$	6.80		Crippen Method
P_c	923.30	kPa	Joback Method
T_{boil}	973.54	K	Joback Method
T_c	1192.35	K	Joback Method
T_{fus}	553.52	K	Joback Method
V_c	1.43	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1244.21	J/mol×K	973.54	Joback Method
η	0.00	Pa×s	973.54	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H42O4/c1-2-3-4-5-6-7-8-9-16-22-29-25(27)19-14-11-15-20-26(28)30-23-21-24-17-12-10-13-18-24/h10,12-13,17-18H,2-9,11,14-16,19-23H2,1H3
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).