Glutaric acid, 1-phenylpropyl undecyl ester

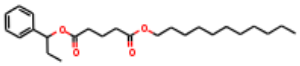
InChI: InChI=1S/C25H40O4/c1-3-5-6-7-8-9-10-11-15-21-28-24(26)19-16-20-25(27)29-23(4-2)22-17-13-12-14-18-22/h12-14,17-18,23H,3-11,15-16,19-21H2,1-2H3

InChI Key: ZHFLSUICMPNRHD-UHFFFAOYSA-N

Formula: C25H40O4

SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)OC(CC)c1ccccc1

Molecular Weight: 404.58



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-198.25	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-817.68	kJ/mol	Joback Method
$\Delta_{fus} H°$	56.60	kJ/mol	Joback Method
$\Delta_{vap} H°$	91.44	kJ/mol	Joback Method
$logP_{oct/wat}$	6.93		Crippen Method
P_c	984.55	kPa	Joback Method
T_{boil}	950.22	K	Joback Method
T_c	1163.44	K	Joback Method
T_{fus}	527.25	K	Joback Method
V_c	1.37	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1182.25	J/mol×K	950.22	Joback Method
η	0.00	Pa×s	950.22	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H40O4/c1-3-5-6-7-8-9-10-11-15-21-28-24(26)19-16-20-25(27)29-23(4-2)22-17-13-12-14-18-22/h12-14,17-18,23H,3-11,15-16,19-21H2,1-2H3
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).