Sebacic acid, hexyl 4-nitrophenyl ester

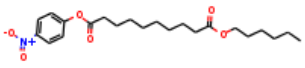
InChI: InChI=1S/C22H33NO6/c1-2-3-4-11-18-28-21(24)12-9-7-5-6-8-10-13-22(25)29-20-16-14-19(15-17-20)23(26)27/h14-17H,2-13,18H2,1H3

InChI Key: BHANGGWDJHMCMJ-UHFFFAOYSA-N

Formula: C22H33NO6

SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1

Molecular Weight: 407.50



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-195.15	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-772.71	kJ/mol	Joback Method
$\Delta_{fus} H°$	63.32	kJ/mol	Joback Method
$\Delta_{vap} H°$	102.41	kJ/mol	Joback Method
$logP_{oct/wat}$	5.74		Crippen Method
P_c	1180.90	kPa	Joback Method
T_{boil}	1038.84	K	Joback Method
T_c	1271.93	K	Joback Method
T_{fus}	664.57	K	Joback Method
V_c	1.29	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1108.40	J/mol×K	1038.84	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C22H33NO6/c1-2-3-4-11-18-28-21(24)12-9-7-5-6-8-10-13-22(25)29-20-16-14-19(15-17-20)23(26)27/h14-17H,2-13,18H2,1H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: 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).