Terephthalic acid, diheptyl ester

Other names: 1,4-Benzenedicarboxylic acid, diheptyl ester.

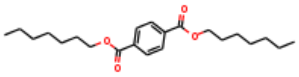
InChI: InChI=1S/C22H34O4/c1-3-5-7-9-11-17-25-21(23)19-13-15-20(16-14-19)22(24)26-18-12-10-8-6-4-2/h13-16H,3-12,17-18H2,1-2H3

InChI Key: RXDQUKGEPHJIJN-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OCCCCCCC)cc1

Molecular Weight: 362.50



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-230.70	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-761.95	kJ/mol	Joback Method
$\Delta_{fus} H°$	51.96	kJ/mol	Joback Method
$\Delta_{vap} H°$	85.82	kJ/mol	Joback Method
$logP_{oct/wat}$	5.94		Crippen Method
P_c	1171.22	kPa	Joback Method
T_{boil}	887.00	K	Joback Method
T_c	1090.20	K	Joback Method
T_{fus}	520.96	K	Joback Method
V_c	1.21	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	997.29	J/mol×K	887.0	Joback Method
η	0.00	Pa×s	887.0	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C22H34O4/c1-3-5-7-9-11-17-25-21(23)19-13-15-20(16-14-19)22(24)26-18-12-10-8-6-4-2/h13-16H,3-12,17-18H2,1-2H3
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).