Phthalic acid, dec-2-yl hexyl ester

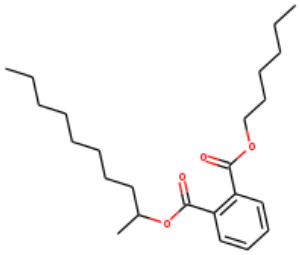
InChI: InChI=1S/C24H38O4/c1-4-6-8-10-11-12-16-20(3)28-24(26)22-18-14-13-17-21(22)23(25)27-19-15-9-7-5-2/h13-14,17-18,20H,4-12,15-16,19H2,1-3H3

InChI Key: HDKBVHRYUCGXQX-UHFFFAOYSA-N

Formula: C24H38O4

SMILES: CCCCCCCCC(C)OC(=O)c1ccccc1C(=O)OCCCCCC

Molecular Weight: 390.56



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-216.30	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-808.51	kJ/mol	Joback Method
$\Delta_{fus} H°$	53.62	kJ/mol	Joback Method
$\Delta_{vap} H°$	89.88	kJ/mol	Joback Method
$logP_{oct/wat}$	6.72		Crippen Method
P_c	1036.57	kPa	Joback Method
T_{boil}	932.32	K	Joback Method
T_c	1142.37	K	Joback Method
T_{fus}	528.50	K	Joback Method
V_c	1.31	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1119.86	J/mol×K	932.32	Joback Method
η	0.00	Pa×s	932.32	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C24H38O4/c1-4-6-8-10-11-12-16-20(3)28-24(26)22-18-14-13-17-21(22)23(25)27-19-15-9-7-5-2/h13-14,17-18,20H,4-12,15-16,19H2,1-3H3

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).