Isophthalic acid, dec-2-yl heptyl ester

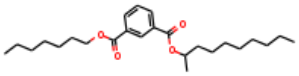
InChI: InChI=1S/C25H40O4/c1-4-6-8-10-11-13-16-21(3)29-25(27)23-18-15-17-22(20-23)24(26)28-19-14-12-9-7-5-2/h15,17-18,20-21H,4-14,16,19H2,1-3H3

InChI Key: KQBAAKXZSCGZJE-UHFFFAOYSA-N

Formula: C25H40O4

SMILES: CCCCCCCCC(C)OC(=O)c1cccc(C(=O)OCCCCCCC)c1

Molecular Weight: 404.58



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-207.88	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-829.15	kJ/mol	Joback Method
$\Delta_{fus} H°$	56.21	kJ/mol	Joback Method
$\Delta_{vap} H°$	92.11	kJ/mol	Joback Method
$logP_{oct/wat}$	7.110		Crippen Method
P_c	975.34	kPa	Joback Method
T_{boil}	955.20	K	Joback Method
T_c	1169.50	K	Joback Method
T_{fus}	539.77	K	Joback Method
V_c	1.369	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1181.72	J/mol×K	955.2	Joback Method
η	0.0000241	Pa×s	955.2	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H40O4/c1-4-6-8-10-11-13-16-21(3)29-25(27)23-18-15-17-22(20-23)24(26)28-19-14-12-9-7-5-2/h15,17-18,20-21H,4-14,16,19H2,1-3H3
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).