Isophthalic acid, hept-2-yl tridecyl ester

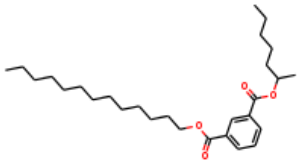
InChI: InChI=1S/C28H46O4/c1-4-6-8-9-10-11-12-13-14-15-17-22-31-27(29)25-20-18-21-26(23-25)28(30)32-24(3)19-16-7-5-2/h18,20-21,23-24H,4-17,19,22H2,1-3H3

InChI Key: BABYNFVXSKVDDR-UHFFFAOYSA-N

Formula: C28H46O4

SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCCCC)c1

Molecular Weight: 446.66



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-182.62	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-891.07	kJ/mol	Joback Method
$\Delta_{fus} H°$	63.98	kJ/mol	Joback Method
$\Delta_{vap} H°$	98.78	kJ/mol	Joback Method
$logP_{oct/wat}$	8.28		Crippen Method
P_c	821.01	kPa	Joback Method
T_{boil}	1023.84	K	Joback Method
T_c	1257.25	K	Joback Method
T_{fus}	573.58	K	Joback Method
V_c	1.54	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1369.87	J/mol×K	1023.84	Joback Method
η	0.00	Pa×s	1023.84	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H46O4/c1-4-6-8-9-10-11-12-13-14-15-17-22-31-27(29)25-20-18-21-26(23-25)28(30)32-24(3)19-16-7-5-2/h18,20-21,23-24H,4-17,19,22H2,1-3H3
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).