Isophthalic acid, 3,3-dimethylbut-2-yl dodecyl ester

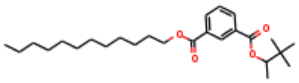
InChI: InChI=1S/C26H42O4/c1-6-7-8-9-10-11-12-13-14-15-19-29-24(27)22-17-16-18-23(20-22)25(28)30-21(2)26(3,4)5/h16-18,20-21H,6-15,19H2,1-5H3

InChI Key: KJOGNTRKUYZRCC-UHFFFAOYSA-N

Formula: C26H42O4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)(C)C)c1

Molecular Weight: 418.61



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-196.62	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-858.54	kJ/mol	Joback Method
$\Delta_{fus} H°$	51.38	kJ/mol	Joback Method
$\Delta_{vap} H°$	93.04	kJ/mol	Joback Method
$logP_{oct/wat}$	7.36		Crippen Method
P_c	930.07	kPa	Joback Method
T_{boil}	974.85	K	Joback Method
T_c	1193.64	K	Joback Method
T_{fus}	553.46	K	Joback Method
V_c	1.41	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1243.96	J/mol×K	974.85	Joback Method
η	0.00	Pa×s	974.85	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H42O4/c1-6-7-8-9-10-11-12-13-14-15-19-29-24(27)22-17-16-18-23(20-22)25(28)30-21(2)26(3,4)5/h16-18,20-21H,6-15,19H2,1-5H3
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).