Phthalic acid, 3-ethylphenyl octyl ester

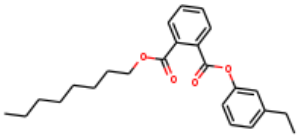
InChI: InChI=1S/C24H30O4/c1-3-5-6-7-8-11-17-27-23(25)21-15-9-10-16-22(21)24(26)28-20-14-12-13-19(4-2)18-20/h9-10,12-16,18H,3-8,11,17H2,1-2H3

InChI Key: QCLMVRZEQCWQKU-UHFFFAOYSA-N

Formula: C24H30O4

SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cccc(CC)c1

Molecular Weight: 382.49



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-111.08	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-578.17	kJ/mol	Joback Method
$\Delta_{fus} H°$	50.79	kJ/mol	Joback Method
$\Delta_{vap} H°$	93.21	kJ/mol	Joback Method
$logP_{oct/wat}$	5.986		Crippen Method
P_c	1277.33	kPa	Joback Method
T_{boil}	964.42	K	Joback Method
T_c	1187.99	K	Joback Method
T_{fus}	582.44	K	Joback Method
V_c	1.212	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1015.71	J/mol×K	964.42	Joback Method
η	0.0000325	Pa×s	964.42	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C24H30O4/c1-3-5-6-7-8-11-17-27-23(25)21-15-9-10-16-22(21)24(26)28-20-14-12-13-19(4-2)18-20/h9-10,12-16,18H,3-8,11,17H2,1-2H3
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).