

Phthalic acid, 3-ethylphenyl octyl ester

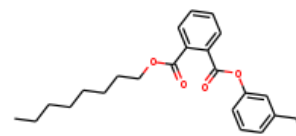
InChI: InChI=1S/C24H30O4/c1-3-5-6-7-8-11-17-27-23(25)21-15-9-10-16-22(21)24(26)28-20-14-12-13-19(4-2)18-20/h9-10,12-16,18H,3-8,11,17H2,1-2H3

InChI Key: QCLMVRZEQCWQKU-UHFFFAOYSA-N

Formula: C₂₄H₃₀O₄

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

Molecular Weight: 382.49



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-111.08	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-578.17	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	50.79	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	93.21	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.99		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	1.21	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1015.71	J/mol×K	964.42	Joback Method
η	0.00	Paxs	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](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

$C_{p, gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: 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 (m³/kg-mol).

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