

Phthalic acid, 3-ethylphenyl octyl ester

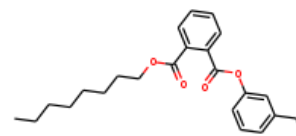
InChI: InChI=1S/C24H30O4/c1-3-5-6-7-8-11-17-27-23(25)21-15-9-10-16-22(21)24(26)28-20-14-12-13-19(4-2)18-20/h9-10,12-16,18H,3-8,11,17H2,1-2H3

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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