# Diethylmalonic acid, octyl 3-phenoxybenzyl ester

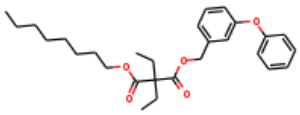
**InChI**: InChI=1S/C28H38O5/c1-4-7-8-9-10-14-20-31-26(29)28(5-2,6-3)27(30)32-22-23-16-15-19-25(21-23)33-24-17-12-11-13-18-24/h11-13,15-19,21H,4-10,14,20,22H2,1-3H3

**InChI Key**: NISSBEZXEKFNNE-UHFFFAOYSA-N

**Formula**: C28H38O5

**SMILES**: CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Oc2ccccc2)c1

**Molecular Weight**: 454.60



## Physical Properties

| Property | Value | Unit | Source |
|---|---|---|---|
| $\Delta_f G°$ | -169.93 | kJ/mol | Joback Method |
| $\Delta_f H°_{gas}$ | -790.23 | kJ/mol | Joback Method |
| $\Delta_{fus} H°$ | 55.32 | kJ/mol | Joback Method |
| $\Delta_{vap} H°$ | 102.56 | kJ/mol | Joback Method |
| $logP_{oct/wat}$ | 7.23 | | Crippen Method |
| $P_c$ | 998.28 | kPa | Joback Method |
| $T_{boil}$ | 1070.15 | K | Joback Method |
| $T_c$ | 1310.17 | K | Joback Method |
| $T_{fus}$ | 639.65 | K | Joback Method |
| $V_c$ | 1.44 | $m^3$/kg-mol | Joback Method |

## Temperature Dependent Properties

| Property | Value | Unit | Temperature (K) | Source |
|---|---|---|---|---|
| $C_{p,gas}$ | 1287.36 | J/mol×K | 1070.15 | Joback Method |
| η | 0.00 | Pa×s | 1070.15 | Joback Method |

## Sources

**Joback Method**: https://en.wikipedia.org/wiki/Joback_method

**NIST Webbook**: http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H38O5/c1-4-7-8-9-10-14-20-31-26(29)28(5-2,6-3)27(30)32-22-23-16-15-19-25(21-23)33-24-17-12-11-13-18-24/h11-13,15-19,21H,4-10,14,20,22H2,1-3H3

**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).