Diethylmalonic acid, pentyl 3-phenoxybenzyl ester

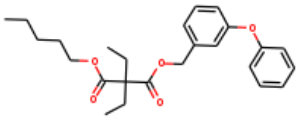
InChI: InChI=1S/C25H32O5/c1-4-7-11-17-28-23(26)25(5-2,6-3)24(27)29-19-20-13-12-16-22(18-20)30-21-14-9-8-10-15-21/h8-10,12-16,18H,4-7,11,17,19H2,1-3H3

InChI Key: WGQMJCWVCDVGSC-UHFFFAOYSA-N

Formula: C25H32O5

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Oc2ccccc2)c1

Molecular Weight: 412.52



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-195.19	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-728.31	kJ/mol	Joback Method
$\Delta_{fus} H°$	47.55	kJ/mol	Joback Method
$\Delta_{vap} H°$	95.88	kJ/mol	Joback Method
$logP_{oct/wat}$	6.06		Crippen Method
P_c	1208.15	kPa	Joback Method
T_{boil}	1001.51	K	Joback Method
T_c	1231.22	K	Joback Method
T_{fus}	605.84	K	Joback Method
V_c	1.27	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1104.59	J/mol×K	1001.51	Joback Method
η	0.00	Pa×s	1001.51	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H32O5/c1-4-7-11-17-28-23(26)25(5-2,6-3)24(27)29-19-20-13-12-16-22(18-20)30-21-14-9-8-10-15-21/h8-10,12-16,18H,4-7,11,17,19H2,1-3H3
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).
$logP_{oct/wat}$: 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 (m^3/kg-mol).