Diethylmalonic acid, 4-bromobenzyl heptyl ester

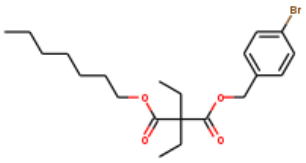
InChI: InChI=1S/C21H31BrO4/c1-4-7-8-9-10-15-25-19(23)21(5-2,6-3)20(24)26-16-17-11-13-18(22)14-12-17/h11-14H,4-10,15-16H2,1-3H3

InChI Key: KEUQDSIGZMYNFA-UHFFFAOYSA-N

Formula: C21H31BrO4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Br)cc1

Molecular Weight: 427.37



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-221.96	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-723.73	kJ/mol	Joback Method
$\Delta_{fus} H°$	47.24	kJ/mol	Joback Method
$\Delta_{vap} H°$	88.73	kJ/mol	Joback Method
$logP_{oct/wat}$	5.81		Crippen Method
P_c	1333.93	kPa	Joback Method
T_{boil}	927.05	K	Joback Method
T_c	1143.73	K	Joback Method
T_{fus}	571.91	K	Joback Method
V_c	1.20	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	978.07	J/mol×K	927.05	Joback Method
η	0.00	Pa×s	927.05	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H31BrO4/c1-4-7-8-9-10-15-25-19(23)21(5-2,6-3)20(24)26-16-17-11-13-18(22)14-12-17/h11-14H,4-10,15-16H2,1-3H3
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).