Sebacic acid, 4-bromophenyl propyl ester

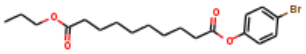
InChI: InChI=1S/C19H27BrO4/c1-2-15-23-18(21)9-7-5-3-4-6-8-10-19(22)24-17-13-11-16(20)12-14-17/h11-14H,2-10,15H2,1H3

InChI Key: PYIZYASZOZGAKK-UHFFFAOYSA-N

Formula: C19H27BrO4

SMILES: CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Br)cc1

Molecular Weight: 399.32



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-241.64	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-673.70	kJ/mol	Joback Method
$\Delta_{fus} H°$	49.48	kJ/mol	Joback Method
$\Delta_{vap} H°$	85.57	kJ/mol	Joback Method
$logP_{oct/wat}$	5.43		Crippen Method
P_c	1519.94	kPa	Joback Method
T_{boil}	884.52	K	Joback Method
T_c	1095.03	K	Joback Method
T_{fus}	546.95	K	Joback Method
V_c	1.10	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	859.35	J/mol×K	884.52	Joback Method
η	0.00	Pa×s	884.52	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H27BrO4/c1-2-15-23-18(21)9-7-5-3-4-6-8-10-19(22)24-17-13-11-16(20)12-14-17/h11-14H,2-10,15H2,1H3
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).