Glutaric acid, hexyl 3-methylbenzyl ester

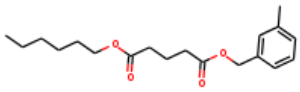
InChI: InChI=1S/C19H28O4/c1-3-4-5-6-13-22-18(20)11-8-12-19(21)23-15-17-10-7-9-16(2)14-17/h7,9-10,14H,3-6,8,11-13,15H2,1-2H3

InChI Key: XBJKVWCXRBBFAG-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCCCCCOC(=O)CCCC(=O)OCc1cccc(C)c1

Molecular Weight: 320.42



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-255.96	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-700.03	kJ/mol	Joback Method
$\Delta_{fus} H°$	44.19	kJ/mol	Joback Method
$\Delta_{vap} H°$	79.14	kJ/mol	Joback Method
$logP_{oct/wat}$	4.33		Crippen Method
P_c	1441.35	kPa	Joback Method
T_{boil}	818.36	K	Joback Method
T_c	1017.87	K	Joback Method
T_{fus}	487.15	K	Joback Method
V_c	1.04	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	819.06	J/mol×K	818.36	Joback Method
η	0.00	Pa×s	818.36	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H28O4/c1-3-4-5-6-13-22-18(20)11-8-12-19(21)23-15-17-10-7-9-16(2)14-17/h7,9-10,14H,3-6,8,11-13,15H2,1-2H3
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).