Glutaric acid, monoamide, N-methyl-N-benzyl-, octyl ester

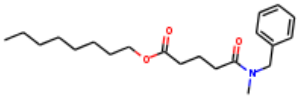
InChI: InChI=1S/C21H33NO3/c1-3-4-5-6-7-11-17-25-21(24)16-12-15-20(23)22(2)18-19-13-9-8-10-14-19/h8-10,13-14H,3-7,11-12,15-18H2,1-2H3

InChI Key: WSYUGFXQPRUZGJ-UHFFFAOYSA-N

Formula: C21H33NO3

SMILES: CCCCCCCCOC(=O)CCCC(=O)N(C)Cc1ccccc1

Molecular Weight: 347.49



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-13.71	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-530.09	kJ/mol	Joback Method
$\Delta_{fus} H°$	51.59	kJ/mol	Joback Method
$\Delta_{vap} H°$	82.56	kJ/mol	Joback Method
$logP_{oct/wat}$	4.72		Crippen Method
P_c	1279.16	kPa	Joback Method
T_{boil}	849.16	K	Joback Method
T_c	1048.11	K	Joback Method
T_{fus}	507.41	K	Joback Method
V_c	1.15	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	950.52	J/mol×K	849.16	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H33NO3/c1-3-4-5-6-7-11-17-25-21(24)16-12-15-20(23)22(2)18-19-13-9-8-10-14-19/h8-10,13-14H,3-7,11-12,15-18H2,1-2H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: 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).
***log*$P_{oct/wat}$**: 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).