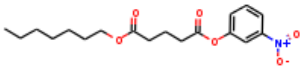
Glutaric acid, heptyl 3-nitrophenyl ester

InChI: InChI=1S/C18H25NO6/c1-2-3-4-5-6-13-24-17(20)11-8-12-18(21)25-16-10-7-9-15(14-16)19(22)23/h7,9-10,14H,2-6,8,11-13H2,1H3
InChI Key: PNOUDIZRSZWHCV-UHFFFAOYSA-N
Formula: C18H25NO6
SMILES: CCCCCCCOC(=O)CCCC(=O)Oc1cccc([N+](=O)[O-])c1
Molecular Weight: 351.39



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-228.83	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-690.15	kJ/mol	Joback Method
$\Delta_{fus} H°$	52.96	kJ/mol	Joback Method
$\Delta_{vap} H°$	93.50	kJ/mol	Joback Method
$logP_{oct/wat}$	4.18		Crippen Method
P_c	1567.23	kPa	Joback Method
T_{boil}	947.32	K	Joback Method
T_c	1169.79	K	Joback Method
T_{fus}	619.49	K	Joback Method
V_c	1.07	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	870.47	J/mol×K	947.32	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H25NO6/c1-2-3-4-5-6-13-24-17(20)11-8-12-18(21)25-16-10-7-9-15(14-16)19(22)23/h7,9-10,14H,2-6,8,11-13H2,1H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: 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).

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