Glutaric acid, heptyl trans-hex-3-enyl ester

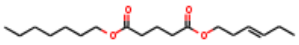
InChI: InChI=1S/C18H32O4/c1-3-5-7-9-11-16-22-18(20)14-12-13-17(19)21-15-10-8-6-4-2/h6,8H,3-5,7,9-16H2,1-2H3/b8-6+

InChI Key: YRGPTAVLLFYUTH-SOFGYWHQSA-N

Formula: C18H32O4

SMILES: CCC=CCCOC(=O)CCCC(=O)OCCCCCCC

Molecular Weight: 312.44



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-286.94	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-787.23	kJ/mol	Joback Method
$\Delta_{fus} H°$	48.15	kJ/mol	Joback Method
$\Delta_{vap} H°$	73.93	kJ/mol	Joback Method
$logP_{oct/wat}$	4.570		Crippen Method
P_c	1273.69	kPa	Joback Method
T_{boil}	767.98	K	Joback Method
T_c	950.09	K	Joback Method
T_{fus}	431.86	K	Joback Method
V_c	1.071	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	825.20	J/mol×K	767.98	Joback Method
η	0.0000612	Pa×s	767.98	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H32O4/c1-3-5-7-9-11-16-22-18(20)14-12-13-17(19)21-15-10-8-6-4-2/h6,8H,3-5,7,9-16H2,1-2H3/b8-6+
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).