

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

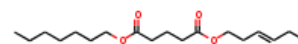
**InChI:** InChI=1S/C18H32O4/c1-3-5-7-9-11-16-22-18(20)14-12-13-17(19)2  
1-15-10-8-6-4-2/h6,8H,3-5,7,9-16H2,1-2H3/b8-6+

**InChI Key:** YRGPTAVLLFYUTH-SOFGYWHQSA-N

**Formula:** C18H32O4

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

**Molecular Weight:** 312.44



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-286.94	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-787.23	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	48.15	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	73.93	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.57		Crippen Method
$P_c$	1273.69	kPa	Joback Method
$T_{\text{boil}}$	767.98	K	Joback Method
$T_c$	950.09	K	Joback Method
$T_{\text{fus}}$	431.86	K	Joback Method
$V_c$	1.07	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	825.20	J/mol×K	767.98	Joback Method
$\eta$	0.00	Paxs	767.98	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/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+](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/ci9903071>

## Legend

$C_{p,gas}$ : Ideal gas heat capacity (J/molxK).

$\eta$ : Dynamic viscosity (Pa $\times$ s).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$ : 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<sup>3</sup>/kg-mol).

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