

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

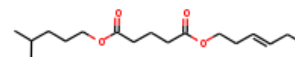
**InChI:** InChI=1S/C17H30O4/c1-4-5-6-7-13-20-16(18)11-8-12-17(19)21-14-9-10-15(2)3/h5-6,15H,4,7-14H2,1-3H3/b6-5+

**InChI Key:** YMRSDUFYLVVVAV-AATRIKPKSA-N

**Formula:** C17H30O4

**SMILES:** CCC=CCCOC(=O)CCCC(=O)OCCCC(C)C

**Molecular Weight:** 298.42



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-297.80	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-771.87	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	42.04	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	71.32	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.04		Crippen Method
$P_c$	1373.78	kPa	Joback Method
$T_{\text{boil}}$	744.66	K	Joback Method
$T_c$	927.57	K	Joback Method
$T_{\text{fus}}$	405.59	K	Joback Method
$V_c$	1.01	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	767.78	J/mol×K	744.66	Joback Method
$\eta$	0.00	Paxs	744.66	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/C17H30O4/c1-4-5-6-7-13-20-16\(18\)11-8-12-17\(19\)21-14-9-10-15\(2\)3/h5-6,15H,4,7-14H2,1-3H3/b6-5+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H30O4/c1-4-5-6-7-13-20-16(18)11-8-12-17(19)21-14-9-10-15(2)3/h5-6,15H,4,7-14H2,1-3H3/b6-5+)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

$\eta$ : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$ : 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).

Latest version available from:

<https://www.cheméo.com/cid/60-048-2/Glutaric%20acid%2C%20isohexyl%20trans-hex-3-enyl%20ester>

Generated by Cheméo on Thu, 22 Mar 2018 17:28:38 +0000.

**Cheméo** (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.