

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

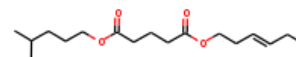
InChI: InChI=1S/C17H30O4/c1-4-5-6-7-13-20-16(18)11-8-12-17(19)21-14-9-10-15(2)3/h5-6,15H,4,7-14H2,1-3H3/b6-5+

InChI Key: YMRSDUFYLVWVAV-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_{boil}	744.66	K	Joback Method
T_c	927.57	K	Joback Method
T_{fus}	405.59	K	Joback Method
V_c	1.01	m ³ /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
η	0.00	Paxs	744.66	Joback Method

Sources

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).

η : 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 (m³/kg-mol).

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