

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

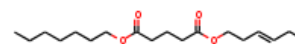
InChI: InChI=1S/C18H32O4/c1-3-5-7-9-11-16-22-18(20)14-12-13-17(19)2
1-15-10-8-6-4-2/h6,8H,3-5,7,9-16H2,1-2H3/b8-6+

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
$\log P_{\text{oct/wat}}$	4.570		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
$C_{p,\text{gas}}$	825.20	J/mol×K	767.98	Joback Method
η	0.0000612	Paxs	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+](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/mol×K).

η : Dynamic viscosity (Pa×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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