

# Sebacic acid, isohexyl pentyl ester

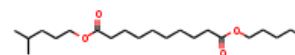
**InChI:** InChI=1S/C21H40O4/c1-4-5-12-17-24-20(22)15-10-8-6-7-9-11-16-21(23)25-18-13-14-19(2)3/h19H,4-18H2,1-3H3

**InChI Key:** PXCSJSVAODQQQL-UHFFFAOYSA-N

**Formula:** C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>

**SMILES:** CCCCCOC(=O)CCCCCCCCC(=O)OCCCC(C)C

**Molecular Weight:** 356.54



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-344.34	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-971.65	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	52.20	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.26	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.82		Crippen Method
$P_c$	1018.13	kPa	Joback Method
$T_{\text{boil}}$	832.02	K	Joback Method
$T_c$	1019.80	K	Joback Method
$T_{\text{fus}}$	455.75	K	Joback Method
$V_c$	1.25	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1030.73	J/mol×K	832.02	Joback Method
$\eta$	0.00	Paxs	832.02	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/C21H40O4/c1-4-5-12-17-24-20\(22\)15-10-8-6-7-9-11-16-21\(23\)25-18-13-14-19\(2\)3/h19H,4-18H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H40O4/c1-4-5-12-17-24-20(22)15-10-8-6-7-9-11-16-21(23)25-18-13-14-19(2)3/h19H,4-18H2,1-3H3)

**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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