

# Sebacic acid, 2,4-dimethylpent-3-yl pentadecyl ester

**InChI:** InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30(33)25-22-19-16-17-20-23-26-31(34)36-32(28(2)3)29(4)5/h28-29,32H,6-27H2,1-5H3

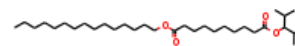
**InChI Key:** IQDRZKWTALQNie-UHFFFAOYSA-N

**Formula:** C<sub>32</sub>H<sub>62</sub>O<sub>4</sub>

**SMILES:**

CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCC(=O)OC(C(C)C)C(C)C

**Molecular Weight:** 510.83



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-256.60	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1209.25	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	73.64	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	103.97	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	9.965		Crippen Method
$P_c$	573.98	kPa	Joback Method
$T_{\text{boil}}$	1082.82	K	Joback Method
$T_c$	1370.02	K	Joback Method
$T_{\text{fus}}$	549.72	K	Joback Method
$V_c$	1.857	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1737.08	J/mol×K	1082.82	Joback Method
$\eta$	0.0000062	Paxs	1082.82	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/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30\(33\)25-22-19-16-17-20-23-26-31\(34\)36-32\(28\(2\)3\)29\(4\)5/h28-29,32H,6-27H2,1-5H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30(33)25-22-19-16-17-20-23-26-31(34)36-32(28(2)3)29(4)5/h28-29,32H,6-27H2,1-5H3)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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).

Latest version available from:

<https://www.chemeo.com/cid/61-035-5/Sebacic%20acid%2C%20%2C4-dimethylpent-3-yl%20pentadecyl%20ester>

Generated by Cheméo on Thu, 19 Jul 2018 07:20:10 +0000.

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