

# 3-Methyl-pent-2-enedioic acid dimethyl ester, Z

**Other names:** cis-2-Pentenedioate, 3-methyl, dimethyl ester.

**InChI:**

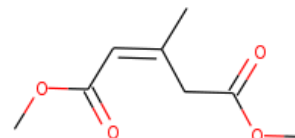
InChI=1S/C8H12O4/c1-6(4-7(9)11-2)5-8(10)12-3/h4H,5H2,1-3H3/b6-4-

**InChI Key:** GBQBEQOEGMZCOH-XQRVVYSFSA-N

**Formula:** C<sub>8</sub>H<sub>12</sub>O<sub>4</sub>

**SMILES:** COC(=O)C=C(C)CC(=O)OC

**Molecular Weight:** 172.18



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-379.69	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-590.62	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	20.94	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.75	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	0.67		Crippen Method
$P_c$	2963.34	kPa	Joback Method
$T_{\text{boil}}$	539.06	K	Joback Method
$T_c$	734.03	K	Joback Method
$T_{\text{fus}}$	305.20	K	Joback Method
$V_c$	0.51	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	303.31	J/mol×K	539.06	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/C8H12O4/c1-6\(4-7\(9\)11-2\)5-8\(10\)12-3/h4H,5H2,1-3H3/b6-4-](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H12O4/c1-6(4-7(9)11-2)5-8(10)12-3/h4H,5H2,1-3H3/b6-4-)

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

## Legend

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

$\Delta_f G^\circ$ : 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).

$\log P_{oct/wat}$ : 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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