# 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-
**InchiKey:** GBQBEQOEGMZCOH-XQRVVYSFSA-N
**Formula:** C8H12O4
**SMILES:** COC(=O)C=C(C)CC(=O)OC
**Mol. weight [g/mol]:** 172.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -379.69 | kJ/mol | Joback Method |
| hf | -590.62 | kJ/mol | Joback Method |
| hfus | 20.94 | kJ/mol | Joback Method |
| hvap | 51.75 | kJ/mol | Joback Method |
| log10ws | -0.75 | | Crippen Method |
| logp | 0.669 | | Crippen Method |
| mcvol | 134.160 | ml/mol | McGowan Method |
| pc | 2963.34 | kPa | Joback Method |
| rinpol | 1162.00 | | NIST Webbook |
| rinpol | 1163.00 | | NIST Webbook |
| rinpol | 1162.00 | | NIST Webbook |
| tb | 539.06 | K | Joback Method |
| tc | 734.03 | K | Joback Method |
| tf | 305.20 | K | Joback Method |
| vc | 0.512 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 303.31 | J/mol×K | 539.06 | Joback Method |
| cpg | 314.42 | J/mol×K | 571.56 | Joback Method |
| cpg | 325.05 | J/mol×K | 604.05 | Joback Method |
| cpg | 335.20 | J/mol×K | 636.55 | Joback Method |
| cpg | 344.87 | J/mol×K | 669.04 | Joback Method |
| cpg | 354.06 | J/mol×K | 701.54 | Joback Method |

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|---|---|---|---|---|
| cpg | 362.77 | J/mol×K | 734.03 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R249117&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |