# 2-Butenoic acid, 2-methyl-, methyl ester

**Other names:** Methyl 2-methyl-2-butenoate
Methyl 2-methylbut-2-enoate
Methyl 2-methylcrotonate
**Inchi:** InChI=1S/C6H10O2/c1-4-5(2)6(7)8-3/h4H,1-3H3/b5-4+
**InchiKey:** YYJWBYNQJLBIGS-SNAWJCMRSA-N
**Formula:** C6H10O2
**SMILES:** CC=C(C)C(=O)OC
**Mol. weight [g/mol]:** 114.14
**CAS:** 41725-90-0

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -162.61 | kJ/mol | Joback Method |
| hf | -304.54 | kJ/mol | Joback Method |
| hfus | 12.97 | kJ/mol | Joback Method |
| hvap | 38.14 | kJ/mol | Joback Method |
| log10ws | -1.05 | | Crippen Method |
| logp | 1.126 | | Crippen Method |
| mcvol | 98.540 | ml/mol | McGowan Method |
| pc | 3497.14 | kPa | Joback Method |
| rinpol | 873.00 | | NIST Webbook |
| ripol | 1184.00 | | NIST Webbook |
| ripol | 1175.00 | | NIST Webbook |
| tb | 417.01 | K | Joback Method |
| tc | 607.33 | K | Joback Method |
| tf | 210.50 | K | Joback Method |
| vc | 0.377 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 184.26 | J/mol×K | 417.01 | Joback Method |
| cpg | 193.90 | J/mol×K | 448.73 | Joback Method |
| cpg | 203.14 | J/mol×K | 480.45 | Joback Method |

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|---|---|---|---|---|
| cpg | 212.00 | J/mol×K | 512.17 | Joback Method |
| cpg | 220.47 | J/mol×K | 543.89 | Joback Method |
| cpg | 228.57 | J/mol×K | 575.61 | Joback Method |
| cpg | 236.31 | J/mol×K | 607.33 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.73866e+01 |
| Coeff. B | -4.35499e+03 |
| Coeff. C | -5.57280e+01 |
| Temperature range (K), min. | 310.37 |
| Temperature range (K), max. | 416.38 |

# Sources

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|---|---|
| **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=C41725900&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **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 |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |