# 2-Butenoic acid, 2-methyl-

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|---|---|
| **Other names:** | Crotonic acid, 2-methyl- |
| | 2-Methyl-2-butenoic acid |
| | CH3CH=C(CH3)COOH |
| | «alpha»-Methylcrotonic acid |
| | 2-Methylcrotonic acid |
| **Inchi:** | InChI=1S/C5H8O2/c1-3-4(2)5(6)7/h3H,1-2H3,(H,6,7) |
| **InchiKey:** | UIERETOOQGIECD-UHFFFAOYSA-N |
| **Formula:** | C5H8O2 |
| **SMILES:** | CC=C(C)C(=O)O |
| **Mol. weight [g/mol]:** | 100.12 |
| **CAS:** | 13201-46-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -202.85 | kJ/mol | Joback Method |
| hf | -303.91 | kJ/mol | Joback Method |
| hfus | 13.29 | kJ/mol | Joback Method |
| hvap | 50.19 | kJ/mol | Joback Method |
| ie | 9.50 | eV | NIST Webbook |
| log10ws | -0.87 | | Crippen Method |
| logp | 1.037 | | Crippen Method |
| mcvol | 84.450 | ml/mol | McGowan Method |
| pc | 4528.58 | kPa | Joback Method |
| rinpol | 934.00 | | NIST Webbook |
| rinpol | 921.00 | | NIST Webbook |
| rinpol | 934.00 | | NIST Webbook |
| rinpol | 921.00 | | NIST Webbook |
| ripol | 1851.00 | | NIST Webbook |
| ripol | 1835.00 | | NIST Webbook |
| ripol | 1808.00 | | NIST Webbook |
| ripol | 1808.00 | | NIST Webbook |
| ripol | 1808.00 | | NIST Webbook |
| tb | 463.89 | K | Joback Method |
| tc | 647.95 | K | Joback Method |
| tf | 343.00 ± 2.00 | K | NIST Webbook |
| vc | 0.322 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 166.62 | J/mol×K | 463.89 | Joback Method |
| cpg | 174.00 | J/mol×K | 494.57 | Joback Method |
| cpg | 181.01 | J/mol×K | 525.24 | Joback Method |
| cpg | 187.67 | J/mol×K | 555.92 | Joback Method |
| cpg | 193.97 | J/mol×K | 586.60 | Joback Method |
| cpg | 199.96 | J/mol×K | 617.27 | Joback Method |
| cpg | 205.63 | J/mol×K | 647.95 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C13201462&Units=SI
**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

# 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
**ie:** Ionization energy
**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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature

| | |
|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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