# 2-Butene, 2-chloro-3-methyl-

**Other names:** 2-Chloro-3-methyl-2-butene
**Inchi:** InChI=1S/C5H9Cl/c1-4(2)5(3)6/h1-3H3
**InchiKey:** WIIKEBDPJPYJHF-UHFFFAOYSA-N
**Formula:** C5H9Cl
**SMILES:** CC(C)=C(C)Cl
**Mol. weight [g/mol]:** 104.58
**CAS:** 17773-65-8

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 42.41 | kJ/mol | Joback Method |
| hf | -64.63 | kJ/mol | Joback Method |
| hfus | 10.48 | kJ/mol | Joback Method |
| hvap | 31.23 | kJ/mol | Joback Method |
| log10ws | -2.42 | | Crippen Method |
| logp | 2.539 | | Crippen Method |
| mcvol | 89.250 | ml/mol | McGowan Method |
| pc | 3572.80 | kPa | Joback Method |
| rinpol | 700.00 | | NIST Webbook |
| rinpol | 698.00 | | NIST Webbook |
| rinpol | 698.00 | | NIST Webbook |
| tb | 355.15 | K | Joback Method |
| tc | 544.94 | K | Joback Method |
| tf | 143.03 | K | Joback Method |
| vc | 0.346 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 137.01 | J/mol×K | 355.15 | Joback Method |
| cpg | 146.03 | J/mol×K | 386.78 | Joback Method |
| cpg | 154.59 | J/mol×K | 418.41 | Joback Method |
| cpg | 162.71 | J/mol×K | 450.04 | Joback Method |
| cpg | 170.41 | J/mol×K | 481.67 | Joback Method |

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|---|---|---|---|---|
| cpg | 177.71 | J/mol×K | 513.31 | Joback Method |
| cpg | 184.63 | J/mol×K | 544.94 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.40196e+01 |
| Coeff. B | -3.13779e+03 |
| Coeff. C | -4.32180e+01 |
| Temperature range (K), min. | 271.72 |
| Temperature range (K), max. | 403.55 |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C17773658&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

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol1758.mol

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |