# Methyl 2-chlorobutanoate

**Other names:** Methyl 2-chlorobutanoate
Methyl 2-chlorobutyrate
**Inchi:** InChI=1S/C5H9ClO2/c1-3-4(6)5(7)8-2/h4H,3H2,1-2H3
**InchiKey:** BHQQXAOBIZQEGI-UHFFFAOYSA-N
**Formula:** C5H9ClO2
**SMILES:** CCC(Cl)C(=O)OC
**Mol. weight [g/mol]:** 136.58

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3725 | | Cheméo Relay (1.0) |
| chl | -2704.00 | kJ/mol | NIST Webbook |
| hf | -505.58 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 12.17 | kJ/mol | Joback Method |
| hvap | 44.87 | kJ/mol | Cheméo Relay (1.0) |
| ie | 10.24 | eV | Cheméo Relay (1.0) |
| log10ws | -1.22 | | Cheméo Relay (1.0) |
| logp | 1.177 | | Crippen Method |
| mcvol | 100.990 | ml/mol | McGowan Method |
| pc | 3538.87 | kPa | Joback Method |
| rinpol | 865.00 | | NIST Webbook |
| rinpol | 875.00 | | NIST Webbook |
| rinpol | 867.00 | | NIST Webbook |
| rinpol | 861.00 | | NIST Webbook |
| rinpol | 859.00 | | NIST Webbook |
| rinpol | 863.00 | | NIST Webbook |
| rinpol | 875.00 | | NIST Webbook |
| rinpol | 863.00 | | NIST Webbook |
| tb | 401.15 | K | Cheméo Relay (1.0) |
| tc | 598.18 | K | Cheméo Relay (1.0) |
| tf | 227.19 | K | Cheméo Relay (1.0) |
| vc | 0.363 | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 186.92 | J/mol×K | 427.08 | Joback Method |
| cpg | 195.50 | J/mol×K | 458.81 | Joback Method |
| cpg | 203.77 | J/mol×K | 490.53 | Joback Method |
| cpg | 211.73 | J/mol×K | 522.26 | Joback Method |
| cpg | 219.39 | J/mol×K | 553.98 | Joback Method |
| cpg | 226.73 | J/mol×K | 585.71 | Joback Method |
| cpg | 233.77 | J/mol×K | 617.43 | Joback Method |
| dvisc | 0.0042591 | Pa×s | 233.19 | Joback Method |
| dvisc | 0.0020958 | Pa×s | 265.50 | Joback Method |
| dvisc | 0.0012028 | Pa×s | 297.82 | Joback Method |
| dvisc | 0.0007696 | Pa×s | 330.13 | Joback Method |
| dvisc | 0.0005332 | Pa×s | 362.45 | Joback Method |
| dvisc | 0.0003923 | Pa×s | 394.76 | Joback Method |
| dvisc | 0.0003024 | Pa×s | 427.08 | Joback Method |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C26464324&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**af:** Acentric Factor
**chl:** Standard liquid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |