# Acetic acid, chloro-, methyl ester

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|---|---|
| **Other names:** | Acetic acid, 2-chloro-, methyl ester |
| | Chloroacetic acid methyl ester |
| | ClH2CCOOCH3 |
| | Methyl chloroacetate |
| | Methyl chloroethanoate |
| | Methyl ester of chloroacetic acid |
| | Methyl monochloracetate |
| | Methyl monochloroacetate |
| | Methylester kyseliny chloroctove |
| | Monochloroacetic acid, methyl ester |
| | NSC 2635 |
| | UN 2295 |
| **Inchi:** | InChI=1S/C3H5ClO2/c1-6-3(5)2-4/h2H2,1H3 |
| **InchiKey:** | QABLOFMHHSOFRJ-UHFFFAOYSA-N |
| **Formula:** | C3H5ClO2 |
| **SMILES:** | COC(=O)CCl |
| **Mol. weight [g/mol]:** | 108.52 |
| **CAS:** | 96-34-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -1451.00 | kJ/mol | NIST Webbook |
| gf | -271.47 | kJ/mol | Joback Method |
| hf | -444.00 ± 10.00 | kJ/mol | NIST Webbook |
| hfl | -487.00 ± 8.80 | kJ/mol | NIST Webbook |
| hfus | 10.51 | kJ/mol | Joback Method |
| hvap | 43.40 ± 4.20 | kJ/mol | NIST Webbook |
| hvap | 46.74 | kJ/mol | NIST Webbook |
| hvap | 46.70 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 46.73 ± 0.06 | kJ/mol | NIST Webbook |
| ie | 10.30 | eV | NIST Webbook |
| ie | 10.53 ± 0.05 | eV | NIST Webbook |
| ie | 10.70 | eV | NIST Webbook |
| log10ws | -0.09 | | Crippen Method |
| logp | 0.398 | | Crippen Method |
| mcvol | 72.810 | ml/mol | McGowan Method |
| pc | 4462.28 | kPa | Joback Method |

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|---|---|---|---|
| rinpol | 731.00 | | NIST Webbook |
| rinpol | 705.00 | | NIST Webbook |
| rinpol | 679.00 | | NIST Webbook |
| rinpol | 691.00 | | NIST Webbook |
| rinpol | 708.00 | | NIST Webbook |
| rinpol | 729.40 | | NIST Webbook |
| ripol | 1318.00 | | NIST Webbook |
| ripol | 1345.00 | | NIST Webbook |
| ripol | 1314.00 | | NIST Webbook |
| ripol | 1270.00 | | NIST Webbook |
| tb | 403.10 ± 0.50 | K | NIST Webbook |
| tb | 403.20 ± 0.50 | K | NIST Webbook |
| tb | 403.10 ± 0.50 | K | NIST Webbook |
| tb | 404.70 ± 0.50 | K | NIST Webbook |
| tb | 400.00 ± 3.00 | K | NIST Webbook |
| tb | 404.00 ± 3.00 | K | NIST Webbook |
| tb | 402.60 | K | NIST Webbook |
| tc | 570.48 | K | Joback Method |
| tf | 241.00 ± 0.02 | K | NIST Webbook |
| tf | 240.50 ± 0.20 | K | NIST Webbook |
| vc | 0.277 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 117.88 | J/mol×K | 381.76 | Joback Method |
| cpg | 123.10 | J/mol×K | 413.21 | Joback Method |
| cpg | 128.19 | J/mol×K | 444.67 | Joback Method |
| cpg | 133.14 | J/mol×K | 476.12 | Joback Method |
| cpg | 137.95 | J/mol×K | 507.57 | Joback Method |
| cpg | 142.60 | J/mol×K | 539.02 | Joback Method |
| cpg | 147.10 | J/mol×K | 570.48 | Joback Method |
| dvisc | 0.0015292 | Pa×s | 251.67 | Joback Method |
| dvisc | 0.0025693 | Pa×s | 225.65 | Joback Method |
| dvisc | 0.0010031 | Pa×s | 277.69 | Joback Method |
| dvisc | 0.0007073 | Pa×s | 303.70 | Joback Method |
| dvisc | 0.0005270 | Pa×s | 329.72 | Joback Method |
| dvisc | 0.0004099 | Pa×s | 355.74 | Joback Method |
| dvisc | 0.0003300 | Pa×s | 381.76 | Joback Method |
| hvapt | 39.23 | kJ/mol | 402.60 | NIST Webbook |
| hvapt | 45.50 | kJ/mol | 360.00 | NIST Webbook |

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|---|---|---|---|---|
| hvapt | 46.70 | kJ/mol | 350.50 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 403.20 | K | 98.70 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.50317e+01 |
| Coeff. B | -3.58037e+03 |
| Coeff. C | -5.91440e+01 |
| Temperature range (K), min. | 301.98 |
| Temperature range (K), max. | 427.49 |

# Sources

**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=C96344&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

# Legend

**chl:** Standard liquid enthalpy of combustion

**cpg:** Ideal gas heat capacity

**dvisc:** Dynamic viscosity

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|---|---|
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |