# Propanoic acid, 2,2-dichloro-, methyl ester

**Other names:** Propionic acid, 2,2-dichloro-, methyl ester
Methyl 2,2-dichloropropionate
2,2-Dichloropropanoic acid methyl ester
**Inchi:** InChI=1S/C4H6Cl2O2/c1-4(5,6)3(7)8-2/h1-2H3
**InchiKey:** RDYUJBOUMXIDPY-UHFFFAOYSA-N
**Formula:** C4H6Cl2O2
**SMILES:** COC(=O)C(C)(Cl)Cl
**Mol. weight [g/mol]:** 157.00
**CAS:** 17640-02-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -272.14 | kJ/mol | Joback Method |
| hf | -410.92 | kJ/mol | Joback Method |
| hfus | 9.88 | kJ/mol | Joback Method |
| hvap | 41.13 | kJ/mol | Joback Method |
| log10ws | -1.27 | | Crippen Method |
| logp | 1.353 | | Crippen Method |
| mcvol | 99.140 | ml/mol | McGowan Method |
| pc | 3853.09 | kPa | Joback Method |
| rinpol | 859.00 | | NIST Webbook |
| rinpol | 854.00 | | NIST Webbook |
| rinpol | 859.00 | | NIST Webbook |
| rinpol | 848.00 | | NIST Webbook |
| rinpol | 859.00 | | NIST Webbook |
| tb | 438.84 | K | Joback Method |
| tc | 646.71 | K | Joback Method |
| tf | 269.26 | K | Joback Method |
| vc | 0.370 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 175.01 | J/mol×K | 438.84 | Joback Method |

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|---|---|---|---|---|
| cpg | 182.58 | J/mol×K | 473.49 | Joback Method |
| cpg | 189.70 | J/mol×K | 508.13 | Joback Method |
| cpg | 196.39 | J/mol×K | 542.78 | Joback Method |
| cpg | 202.66 | J/mol×K | 577.42 | Joback Method |
| cpg | 208.52 | J/mol×K | 612.07 | Joback Method |
| cpg | 213.99 | J/mol×K | 646.71 | Joback Method |
| dvisc | 0.0038664 | Pa×s | 269.26 | Joback Method |
| dvisc | 0.0021689 | Pa×s | 297.52 | Joback Method |
| dvisc | 0.0013451 | Pa×s | 325.79 | Joback Method |
| dvisc | 0.0009003 | Pa×s | 354.05 | Joback Method |
| dvisc | 0.0006394 | Pa×s | 382.31 | Joback Method |
| dvisc | 0.0004761 | Pa×s | 410.58 | Joback Method |
| dvisc | 0.0003682 | Pa×s | 438.84 | Joback Method |

# 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=C17640027&Units=SI

# Legend

**cpg:** Ideal gas heat capacity

**dvisc:** Dynamic viscosity

**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

**rinpol:** Non-polar retention indices

**tb:** Normal Boiling Point Temperature

**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume