# Dichloroacetic acid, allyl ester

**Other names:** Allyl dichloroacetate
2-Propen-1-ol, dichloroacetate
**Inchi:** InChI=1S/C5H6Cl2O2/c1-2-3-9-5(8)4(6)7/h2,4H,1,3H2
**InchiKey:** UJUPTENXDPFFDP-UHFFFAOYSA-N
**Formula:** C5H6Cl2O2
**SMILES:** C=CCOC(=O)C(Cl)Cl
**Mol. weight [g/mol]:** 169.01
**CAS:** 30895-77-3

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -2479.00 | kJ/mol | NIST Webbook |
| chl | -2925.00 ± 3.00 | kJ/mol | NIST Webbook |
| gf | -181.16 | kJ/mol | Joback Method |
| hf | -302.66 | kJ/mol | Joback Method |
| hfus | 15.08 | kJ/mol | Joback Method |
| hvap | 43.59 | kJ/mol | Joback Method |
| log10ws | -1.54 | | Crippen Method |
| logp | 1.519 | | Crippen Method |
| mcvol | 108.930 | ml/mol | McGowan Method |
| pc | 3560.02 | kPa | Joback Method |
| rinpol | 946.00 | | NIST Webbook |
| rinpol | 946.00 | | NIST Webbook |
| rinpol | 946.00 | | NIST Webbook |
| ripol | 1504.00 | | NIST Webbook |
| tb | 461.19 | K | Joback Method |
| tc | 662.38 | K | Joback Method |
| tf | 261.35 | K | Joback Method |
| vc | 0.412 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 193.30 | J/mol×K | 461.19 | Joback Method |

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|---|---|---|---|---|
| cpg | 227.24 | J/mol×K | 628.85 | Joback Method |
| cpg | 221.14 | J/mol×K | 595.32 | Joback Method |
| cpg | 214.70 | J/mol×K | 561.79 | Joback Method |
| cpg | 207.92 | J/mol×K | 528.25 | Joback Method |
| cpg | 200.79 | J/mol×K | 494.72 | Joback Method |
| cpg | 233.00 | J/mol×K | 662.38 | Joback Method |
| dvisc | 0.0003182 | Pa×s | 461.19 | Joback Method |
| dvisc | 0.0004074 | Pa×s | 427.88 | Joback Method |
| dvisc | 0.0005439 | Pa×s | 394.58 | Joback Method |
| dvisc | 0.0007659 | Pa×s | 361.27 | Joback Method |
| dvisc | 0.0011562 | Pa×s | 327.96 | Joback Method |
| dvisc | 0.0019155 | Pa×s | 294.66 | Joback Method |
| dvisc | 0.0036093 | Pa×s | 261.35 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C30895773&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 |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |

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