# Dichloroacetaldehyde

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|---|---|
| **Other names:** | 2,2-DICHLOROACETALDEHYDE |
| | Acetaldehyde, 2,2-dichloro- |
| | Acetaldehyde,dichloro- |
| | CHCl2CHO |
| | CHLOROALDEHYDE |
| | Chloraldehyde |
| | «alpha»,«alpha»-Dichloroacetaldehyde |
| | Â«alphaÂ»,Â«alphaÂ»-Dichloroacetaldehyde |
| **Inchi:** | InChI=1S/C2H2Cl2O/c3-2(4)1-5/h1-2H |
| **InchiKey:** | NWQWQKUXRJYXFH-UHFFFAOYSA-N |
| **Formula:** | C2H2Cl2O |
| **SMILES:** | O=CC(Cl)Cl |
| **Mol. weight [g/mol]:** | 112.94 |
| **CAS:** | 79-02-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -159.86 | kJ/mol | Joback Method |
| hf | -206.95 | kJ/mol | Joback Method |
| hfus | 8.10 | kJ/mol | Joback Method |
| hvap | 35.15 | kJ/mol | Joback Method |
| log10ws | -0.85 | | Crippen Method |
| logp | 0.989 | | Crippen Method |
| mcvol | 65.090 | ml/mol | McGowan Method |
| pc | 5087.49 | kPa | Joback Method |
| tb | 368.24 | K | Joback Method |
| tc | 565.66 | K | Joback Method |
| tf | 199.14 | K | Joback Method |
| vc | 0.257 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 90.58 | J/mol×K | 368.24 | Joback Method |

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|---|---|---|---|---|
| cpg | 94.08 | J/mol×K | 401.14 | Joback Method |
| cpg | 97.39 | J/mol×K | 434.05 | Joback Method |
| cpg | 100.51 | J/mol×K | 466.95 | Joback Method |
| cpg | 103.46 | J/mol×K | 499.85 | Joback Method |
| cpg | 106.23 | J/mol×K | 532.75 | Joback Method |
| cpg | 108.83 | J/mol×K | 565.66 | Joback Method |
| dvisc | 0.0052647 | Pa×s | 199.14 | Joback Method |
| dvisc | 0.0027013 | Pa×s | 227.32 | Joback Method |
| dvisc | 0.0016058 | Pa×s | 255.51 | Joback Method |
| dvisc | 0.0010585 | Pa×s | 283.69 | Joback Method |
| dvisc | 0.0007524 | Pa×s | 311.87 | Joback Method |
| dvisc | 0.0005659 | Pa×s | 340.06 | Joback Method |
| dvisc | 0.0004446 | Pa×s | 368.24 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.46568e+01 |
| Coeff. B | -3.17177e+03 |
| Coeff. C | -4.77390e+01 |
| Temperature range (K), min. | 268.47 |
| Temperature range (K), max. | 387.13 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 8.23568e+01 |
| Coeff. B | -7.19495e+03 |
| Coeff. C | -9.97640e+00 |
| Coeff. D | 6.95470e-06 |
| Temperature range (K), min. | 223.00 |
| Temperature range (K), max. | 555.00 |

# Sources

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|---|---|
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1773 |
| **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/mol1773.mol |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C79027&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

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