# Acetyl chloride, chloro-

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|---|---|
| **Other names:** | ALPHA-CHLOROACETYL CHLORIDE |
| | Acetyl chloride, 2-chloro- |
| | CH2ClCOCl |
| | CHLOROACETIC ACID CHLORIDE |
| | Chloracetyl chloride |
| | Chlorid kyseliny chloroctove |
| | Chloroacetic chloride |
| | Chloroacetyl chloride |
| | Chloroethanoyl chloride |
| | Chlorure de chloracetyle |
| | Monochloroacetyl chloride |
| | UN 1752 |
| | «alpha»-Chloroacetyl chloride |
| | Â«alphaÂ»-Chloroacetyl chloride |
| **Inchi:** | InChI=1S/C2H2Cl2O/c3-1-2(4)5/h1H2 |
| **InchiKey:** | VGCXGMAHQTYDJK-UHFFFAOYSA-N |
| **Formula:** | C2H2Cl2O |
| **SMILES:** | O=C(Cl)CCl |
| **Mol. weight [g/mol]:** | 112.94 |
| **CAS:** | 79-04-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -186.82 | kJ/mol | Joback Method |
| hf | -246.00 ± 8.80 | kJ/mol | NIST Webbook |
| hfl | -285.00 ± 8.40 | kJ/mol | NIST Webbook |
| hfus | 10.93 | kJ/mol | Joback Method |
| hvap | 35.56 | kJ/mol | Joback Method |
| ie | 10.30 | eV | NIST Webbook |
| log10ws | -0.74 | | Crippen Method |
| logp | 0.991 | | Crippen Method |
| mcvol | 65.090 | ml/mol | McGowan Method |
| pc | 4952.36 | kPa | Joback Method |
| rinpol | 622.00 | | NIST Webbook |
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| rinpol | 622.00 | | NIST Webbook |
| tb | 373.89 | K | Joback Method |

| | | | |
|---|---|---|---|
| tc | 572.48 | K | Joback Method |
| tf | 377.00 | K | NIST Webbook |
| tf | 251.38 ± 0.07 | K | NIST Webbook |
| vc | 0.252 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 87.44 | J/mol×K | 373.89 | Joback Method |
| cpg | 90.94 | J/mol×K | 406.99 | Joback Method |
| cpg | 94.26 | J/mol×K | 440.09 | Joback Method |
| cpg | 97.40 | J/mol×K | 473.19 | Joback Method |
| cpg | 100.38 | J/mol×K | 506.28 | Joback Method |
| cpg | 103.20 | J/mol×K | 539.38 | Joback Method |
| cpg | 105.86 | J/mol×K | 572.48 | Joback Method |
| dvisc | 0.0019197 | Pa×s | 247.37 | Joback Method |
| dvisc | 0.0031682 | Pa×s | 222.07 | Joback Method |
| dvisc | 0.0012766 | Pa×s | 272.68 | Joback Method |
| dvisc | 0.0009098 | Pa×s | 297.98 | Joback Method |
| dvisc | 0.0006838 | Pa×s | 323.28 | Joback Method |
| dvisc | 0.0005356 | Pa×s | 348.59 | Joback Method |
| dvisc | 0.0004337 | Pa×s | 373.89 | Joback Method |
| hvapt | 45.00 | kJ/mol | 316.00 | NIST Webbook |
| hvapt | 40.80 | kJ/mol | 340.50 | NIST Webbook |
| hvapt | 44.10 | kJ/mol | 331.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.47993e+01 |
| Coeff. B | -3.27151e+03 |
| Coeff. C | -5.76630e+01 |
| Temperature range (K), min. | 283.10 |
| Temperature range (K), max. | 402.68 |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C79049&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **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/mol1772.mol |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |