# Ethyne, chloro-

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|---|---|
| **Other names:** | 1-Chloroacetylene |
| | Acetylene, chloro- |
| | C2HCl |
| | Chloroacetylene |
| | Chloroethyne |
| | Ethynyl chloride |
| | Monochloroacetylene |
| **Inchi:** | InChI=1S/C2HCl/c1-2-3/h1H |
| **InchiKey:** | DIWKDXFZXXCDLF-UHFFFAOYSA-N |
| **Formula:** | C2HCl |
| **SMILES:** | C#CCl |
| **Mol. weight [g/mol]:** | 60.48 |
| **CAS:** | 593-63-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 177.10 | kJ/mol | Joback Method |
| hf | 226.00 ± 10.00 | kJ/mol | NIST Webbook |
| hfl | 207.00 ± 10.00 | kJ/mol | NIST Webbook |
| hfus | 8.11 | kJ/mol | Joback Method |
| hvap | 20.00 ± 1.00 | kJ/mol | NIST Webbook |
| ie | 10.58 ± 0.02 | eV | NIST Webbook |
| ie | 11.04 ± 0.00 | eV | NIST Webbook |
| ie | 10.70 ± 0.10 | eV | NIST Webbook |
| ie | 10.63 | eV | NIST Webbook |
| ie | 10.60 | eV | NIST Webbook |
| ie | 10.60 ± 0.02 | eV | NIST Webbook |
| log10ws | -1.10 | | Crippen Method |
| logp | 0.816 | | Crippen Method |
| mcvol | 42.680 | ml/mol | McGowan Method |
| pc | 5926.27 | kPa | Joback Method |
| rinpol | 320.00 | | NIST Webbook |
| tb | 272.71 | K | Joback Method |
| tc | 455.70 | K | Joback Method |
| tf | 189.19 | K | Joback Method |
| vc | 0.159 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 50.11 | J/mol×K | 272.71 | Joback Method |
| cpg | 51.89 | J/mol×K | 303.21 | Joback Method |
| cpg | 53.55 | J/mol×K | 333.71 | Joback Method |
| cpg | 55.09 | J/mol×K | 364.21 | Joback Method |
| cpg | 56.53 | J/mol×K | 394.71 | Joback Method |
| cpg | 57.86 | J/mol×K | 425.20 | Joback Method |
| cpg | 59.11 | J/mol×K | 455.70 | Joback Method |
| hvapt | 21.80 | kJ/mol | 221.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 8.62630e+00 |
| Coeff. B | -9.57465e+02 |
| Coeff. C | -4.58380e+01 |
| Temperature range (K), min. | 160.66 |
| Temperature range (K), max. | 334.68 |

# Sources

| | |
|---|---|
| **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=C593635&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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |