# Pentane, 3-chloro-

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|---|---|
| **Other names:** | 1-Ethylpropyl chloride |
| | 3-Chloropentane |
| **Inchi:** | InChI=1S/C5H11Cl/c1-3-5(6)4-2/h5H,3-4H2,1-2H3 |
| **InchiKey:** | CXQSCYIVCSCSES-UHFFFAOYSA-N |
| **Formula:** | C5H11Cl |
| **SMILES:** | CCC(Cl)CC |
| **Mol. weight [g/mol]:** | 106.59 |
| **CAS:** | 616-20-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -23.15 | kJ/mol | Joback Method |
| hf | -167.55 | kJ/mol | Joback Method |
| hfus | 9.38 | kJ/mol | Joback Method |
| hvap | 30.72 | kJ/mol | Joback Method |
| log10ws | -2.63 | | Aqueous Solubility Prediction Method |
| logp | 2.414 | | Crippen Method |
| mcvol | 93.550 | ml/mol | McGowan Method |
| pc | 3352.86 | kPa | Joback Method |
| rinpol | 706.00 | | NIST Webbook |
| rinpol | 721.00 | | NIST Webbook |
| rinpol | 706.00 | | NIST Webbook |
| rinpol | 721.00 | | NIST Webbook |
| rinpol | 695.00 | | NIST Webbook |
| ripol | 878.00 | | NIST Webbook |
| ripol | 892.00 | | NIST Webbook |
| ripol | 900.00 | | NIST Webbook |
| ripol | 880.00 | | NIST Webbook |
| tb | 368.05 ± 2.00 | K | NIST Webbook |
| tb | 370.94 ± 0.30 | K | NIST Webbook |
| tb | 370.65 ± 4.00 | K | NIST Webbook |
| tb | 370.70 | K | NIST Webbook |
| tc | 527.49 | K | Joback Method |
| tf | 168.00 ± 2.00 | K | NIST Webbook |
| tf | 168.00 ± 2.00 | K | NIST Webbook |
| vc | 0.358 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 201.54 | J/mol×K | 527.49 | Joback Method |
| cpg | 193.96 | J/mol×K | 498.04 | Joback Method |
| cpg | 186.05 | J/mol×K | 468.59 | Joback Method |
| cpg | 177.80 | J/mol×K | 439.14 | Joback Method |
| cpg | 169.22 | J/mol×K | 409.69 | Joback Method |
| cpg | 160.28 | J/mol×K | 380.24 | Joback Method |
| cpg | 150.99 | J/mol×K | 350.79 | Joback Method |
| dvisc | 0.0078623 | Pa×s | 161.03 | Joback Method |
| dvisc | 0.0002823 | Pa×s | 350.79 | Joback Method |
| dvisc | 0.0003734 | Pa×s | 319.16 | Joback Method |
| dvisc | 0.0005253 | Pa×s | 287.54 | Joback Method |
| dvisc | 0.0008040 | Pa×s | 255.91 | Joback Method |
| dvisc | 0.0013876 | Pa×s | 224.28 | Joback Method |
| dvisc | 0.0028647 | Pa×s | 192.66 | Joback Method |
| hvapt | 36.50 | kJ/mol | 349.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.40997e+01 |
| Coeff. B | -3.01495e+03 |
| Coeff. C | -5.27140e+01 |
| Temperature range (K), min. | 271.00 |
| Temperature range (K), max. | 395.78 |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C616206&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |