# Heptane, 3-chloro-2-methyl

**Other names:** 3-Chloro-2-methylheptane
**Inchi:** InChI=1S/C8H17Cl/c1-4-5-6-8(9)7(2)3/h7-8H,4-6H2,1-3H3
**InchiKey:** YDUVDHAEYHZJQQ-UHFFFAOYSA-N
**Formula:** C8H17Cl
**SMILES:** CCCCC(Cl)C(C)C
**Mol. weight [g/mol]:** 148.67
**CAS:** ---

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -0.33 | kJ/mol | Joback Method |
| hf | -234.75 | kJ/mol | Joback Method |
| hfus | 13.63 | kJ/mol | Joback Method |
| hvap | 37.01 | kJ/mol | Joback Method |
| log10ws | -3.19 | | Crippen Method |
| logp | 3.440 | | Crippen Method |
| mcvol | 135.820 | ml/mol | McGowan Method |
| pc | 2482.59 | kPa | Joback Method |
| rinpol | 947.00 | | NIST Webbook |
| rinpol | 947.00 | | NIST Webbook |
| rinpol | 947.00 | | NIST Webbook |
| tb | 418.99 | K | Joback Method |
| tc | 597.64 | K | Joback Method |
| tf | 179.84 | K | Joback Method |
| vc | 0.520 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 262.83 | J/mol×K | 418.99 | Joback Method |
| cpg | 325.02 | J/mol×K | 567.87 | Joback Method |
| cpg | 313.63 | J/mol×K | 538.09 | Joback Method |
| cpg | 301.74 | J/mol×K | 508.32 | Joback Method |
| cpg | 289.32 | J/mol×K | 478.54 | Joback Method |

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|---|---|---|---|---|
| cpg | 276.35 | J/mol×K | 448.77 | Joback Method |
| cpg | 335.90 | J/mol×K | 597.64 | Joback Method |
| dvisc | 0.0002571 | Pa×s | 418.99 | Joback Method |
| dvisc | 0.0003572 | Pa×s | 379.13 | Joback Method |
| dvisc | 0.0005362 | Pa×s | 339.27 | Joback Method |
| dvisc | 0.0008967 | Pa×s | 299.42 | Joback Method |
| dvisc | 0.0017563 | Pa×s | 259.56 | Joback Method |
| dvisc | 0.0043901 | Pa×s | 219.70 | Joback Method |
| dvisc | 0.0164704 | Pa×s | 179.84 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.39315e+01 |
| Coeff. B | -3.62925e+03 |
| Coeff. C | -6.21220e+01 |
| Temperature range (K), min. | 328.12 |
| Temperature range (K), max. | 483.15 |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**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=R116017&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

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |