# Pentane, 1-chloro-2-methyl

**Inchi:** InChI=1S/C6H13Cl/c1-3-4-6(2)5-7/h6H,3-5H2,1-2H3
**InchiKey:** SLBTUZZYJLBZQV-UHFFFAOYSA-N
**Formula:** C6H13Cl
**SMILES:** CCCC(C)CCl
**Mol. weight [g/mol]:** 120.62

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -14.73 | kJ/mol | Joback Method |
| hf | -188.19 | kJ/mol | Joback Method |
| hfus | 11.97 | kJ/mol | Joback Method |
| hvap | 32.95 | kJ/mol | Joback Method |
| log10ws | -2.25 | | Crippen Method |
| logp | 2.661 | | Crippen Method |
| mcvol | 107.640 | ml/mol | McGowan Method |
| pc | 3009.03 | kPa | Joback Method |
| rinpol | 823.00 | | NIST Webbook |
| rinpol | 823.00 | | NIST Webbook |
| rinpol | 823.00 | | NIST Webbook |
| rinpol | 867.00 | | NIST Webbook |
| rinpol | 880.00 | | NIST Webbook |
| rinpol | 871.00 | | NIST Webbook |
| rinpol | 871.00 | | NIST Webbook |
| ripol | 988.00 | | NIST Webbook |
| ripol | 988.00 | | NIST Webbook |
| ripol | 979.00 | | NIST Webbook |
| ripol | 1000.00 | | NIST Webbook |
| tb | 373.67 | K | Joback Method |
| tc | 550.01 | K | Joback Method |
| tf | 172.30 | K | Joback Method |
| vc | 0.414 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 185.85 | J/mol×K | 373.67 | Joback Method |
| cpg | 196.56 | J/mol×K | 403.06 | Joback Method |
| cpg | 206.84 | J/mol×K | 432.45 | Joback Method |
| cpg | 216.72 | J/mol×K | 461.84 | Joback Method |
| cpg | 226.20 | J/mol×K | 491.23 | Joback Method |
| cpg | 235.29 | J/mol×K | 520.62 | Joback Method |
| cpg | 244.00 | J/mol×K | 550.01 | Joback Method |
| dvisc | 0.0084225 | Pa×s | 172.30 | Joback Method |
| dvisc | 0.0030184 | Pa×s | 205.86 | Joback Method |
| dvisc | 0.0014423 | Pa×s | 239.42 | Joback Method |
| dvisc | 0.0008264 | Pa×s | 272.99 | Joback Method |
| dvisc | 0.0005349 | Pa×s | 306.55 | Joback Method |
| dvisc | 0.0003773 | Pa×s | 340.11 | Joback Method |
| dvisc | 0.0002833 | Pa×s | 373.67 | Joback Method |

# 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=R32688&Units=SI
**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
**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 |