# 3-Pentanol, 1-chloro-3-methyl-

**Inchi:** InChI=1S/C6H13ClO/c1-3-6(2,8)4-5-7/h8H,3-5H2,1-2H3
**InchiKey:** IPPWCUJAYBWKFJ-UHFFFAOYSA-N
**Formula:** C6H13ClO
**SMILES:** CCC(C)(O)CCCl
**Mol. weight [g/mol]:** 136.62
**CAS:** 33879-66-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -146.27 | kJ/mol | Joback Method |
| hf | -343.89 | kJ/mol | Joback Method |
| hfus | 12.17 | kJ/mol | Joback Method |
| hvap | 48.72 | kJ/mol | Joback Method |
| log10ws | -1.86 | | Crippen Method |
| logp | 1.776 | | Crippen Method |
| mcvol | 113.510 | ml/mol | McGowan Method |
| pc | 3380.21 | kPa | Joback Method |
| tb | 463.06 | K | Joback Method |
| tc | 640.48 | K | Joback Method |
| tf | 250.54 | K | Joback Method |
| vc | 0.428 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 236.38 | J/mol×K | 463.06 | Joback Method |
| cpg | 281.88 | J/mol×K | 610.91 | Joback Method |
| cpg | 273.74 | J/mol×K | 581.34 | Joback Method |
| cpg | 265.15 | J/mol×K | 551.77 | Joback Method |
| cpg | 256.07 | J/mol×K | 522.20 | Joback Method |
| cpg | 246.49 | J/mol×K | 492.63 | Joback Method |
| cpg | 289.58 | J/mol×K | 640.48 | Joback Method |
| dvisc | 0.0002270 | Pa×s | 463.06 | Joback Method |
| dvisc | 0.0003888 | Pa×s | 427.64 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0007336 | Pa×s | 392.22 | Joback Method |
| dvisc | 0.0015703 | Pa×s | 356.80 | Joback Method |
| dvisc | 0.0039750 | Pa×s | 321.38 | Joback Method |
| dvisc | 0.0126658 | Pa×s | 285.96 | Joback Method |
| dvisc | 0.0560055 | Pa×s | 250.54 | 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=C33879662&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |