# 1-chloro-1-propanol

**Inchi:** InChI=1S/C3H7ClO/c1-2-3(4)5/h3,5H,2H2,1H3
**InchiKey:** RZWHKKIXMPLQEM-UHFFFAOYSA-N
**Formula:** C3H7ClO
**SMILES:** CCC(O)Cl
**Mol. weight [g/mol]:** 94.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -176.81 | kJ/mol | Joback Method |
| hf | -278.50 | kJ/mol | Joback Method |
| hfus | 8.29 | kJ/mol | Joback Method |
| hvap | 42.95 | kJ/mol | Joback Method |
| log10ws | -1.10 | | Crippen Method |
| logp | 0.954 | | Crippen Method |
| mcvol | 71.240 | ml/mol | McGowan Method |
| pc | 4802.50 | kPa | Joback Method |
| rinpol | 678.00 | | NIST Webbook |
| rinpol | 678.00 | | NIST Webbook |
| tb | 397.21 | K | Joback Method |
| tc | 571.23 | K | Joback Method |
| tf | 199.31 | K | Joback Method |
| vc | 0.266 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 122.10 | J/mol×K | 397.21 | Joback Method |
| cpg | 148.55 | J/mol×K | 542.23 | Joback Method |
| cpg | 143.70 | J/mol×K | 513.23 | Joback Method |
| cpg | 138.64 | J/mol×K | 484.22 | Joback Method |
| cpg | 133.36 | J/mol×K | 455.22 | Joback Method |
| cpg | 127.85 | J/mol×K | 426.21 | Joback Method |
| cpg | 153.19 | J/mol×K | 571.23 | Joback Method |
| dvisc | 0.0003683 | Pa×s | 397.21 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0006545 | Pa×s | 364.23 | Joback Method |
| dvisc | 0.0013040 | Pa×s | 331.24 | Joback Method |
| dvisc | 0.0030263 | Pa×s | 298.26 | Joback Method |
| dvisc | 0.0086584 | Pa×s | 265.28 | Joback Method |
| dvisc | 0.0333896 | Pa×s | 232.29 | Joback Method |
| dvisc | 0.2012782 | Pa×s | 199.31 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R216236&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |