# 2-Chlorobutyramide

**Inchi:** InChI=1S/C4H8ClNO/c1-2-3(5)4(6)7/h3H,2H2,1H3,(H2,6,7)
**InchiKey:** VJIOSCMTZVXQQU-UHFFFAOYSA-N
**Formula:** C4H8ClNO
**SMILES:** CCC(Cl)C(N)=O
**Mol. weight [g/mol]:** 121.56
**CAS:** 7462-73-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -94.04 | kJ/mol | Joback Method |
| hf | -225.70 | kJ/mol | Joback Method |
| hfus | 13.59 | kJ/mol | Joback Method |
| hvap | 45.88 | kJ/mol | Joback Method |
| log10ws | -0.97 | | Crippen Method |
| logp | 0.489 | | Crippen Method |
| mcvol | 91.010 | ml/mol | McGowan Method |
| pc | 4379.97 | kPa | Joback Method |
| tb | 454.31 | K | Joback Method |
| tc | 661.30 | K | Joback Method |
| tf | 282.95 | K | Joback Method |
| vc | 0.338 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 174.28 | J/mol×K | 454.31 | Joback Method |
| cpg | 182.33 | J/mol×K | 488.81 | Joback Method |
| cpg | 189.97 | J/mol×K | 523.31 | Joback Method |
| cpg | 197.21 | J/mol×K | 557.81 | Joback Method |
| cpg | 204.05 | J/mol×K | 592.31 | Joback Method |
| cpg | 210.52 | J/mol×K | 626.81 | Joback Method |
| cpg | 216.63 | J/mol×K | 661.30 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C7462739&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |