# Acetanilide, 2'-carbamoyl-2-chloro-

**Inchi:** InChI=1S/C9H9ClN2O2/c10-5-8(13)12-7-4-2-1-3-6(7)9(11)14/h1-4H,5H2,(H2,11,14)(H,12
**InchiKey:** LCDQTZCLXUMOGO-UHFFFAOYSA-N
**Formula:** C9H9ClN2O2
**SMILES:** NC(=O)c1ccccc1NC(=O)CCl
**Mol. weight [g/mol]:** 212.63
**CAS:** 21721-78-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 13.75 | kJ/mol | Joback Method |
| hf | -157.67 | kJ/mol | Joback Method |
| hfus | 30.41 | kJ/mol | Joback Method |
| hvap | 73.52 | kJ/mol | Joback Method |
| log10ws | -2.00 | | Crippen Method |
| logp | 0.963 | | Crippen Method |
| mcvol | 149.250 | ml/mol | McGowan Method |
| pc | 3872.29 | kPa | Joback Method |
| tb | 704.85 | K | Joback Method |
| tc | 942.04 | K | Joback Method |
| tf | 495.83 | K | Joback Method |
| vc | 0.556 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 365.70 | J/mol×K | 704.85 | Joback Method |
| cpg | 375.54 | J/mol×K | 744.38 | Joback Method |
| cpg | 384.57 | J/mol×K | 783.91 | Joback Method |
| cpg | 392.83 | J/mol×K | 823.45 | Joback Method |
| cpg | 400.34 | J/mol×K | 862.98 | Joback Method |
| cpg | 407.16 | J/mol×K | 902.51 | Joback Method |
| cpg | 413.32 | J/mol×K | 942.04 | Joback Method |

# Sources

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|---|---|
| **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=C21721788&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |