# Acetanilide, 2',4'-diamino

**Other names:** N-(2,4-diaminophenyl)acetamide
**Inchi:** InChI=1S/C8H11N3O/c1-5(12)11-8-3-2-6(9)4-7(8)10/h2-4H,9-10H2,1H3,(H,11,12)
**InchiKey:** XLXOPVQPBPLVHP-UHFFFAOYSA-N
**Formula:** C8H11N3O
**SMILES:** CC(=O)Nc1ccc(N)cc1N
**Mol. weight [g/mol]:** 165.19
**CAS:** 6373-15-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 203.00 | kJ/mol | Joback Method |
| hf | 13.61 | kJ/mol | Joback Method |
| hfus | 26.83 | kJ/mol | Joback Method |
| hvap | 71.47 | kJ/mol | Joback Method |
| log10ws | -0.94 | | Crippen Method |
| logp | 0.809 | | Crippen Method |
| mcvol | 131.330 | ml/mol | McGowan Method |
| pc | 4474.22 | kPa | Joback Method |
| tb | 668.18 | K | Joback Method |
| tc | 908.23 | K | Joback Method |
| tf | 500.49 | K | Joback Method |
| vc | 0.474 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 337.47 | J/mol×K | 668.18 | Joback Method |
| cpg | 348.30 | J/mol×K | 708.19 | Joback Method |
| cpg | 358.34 | J/mol×K | 748.20 | Joback Method |
| cpg | 367.62 | J/mol×K | 788.20 | Joback Method |
| cpg | 376.16 | J/mol×K | 828.21 | Joback Method |
| cpg | 384.01 | J/mol×K | 868.22 | Joback Method |
| cpg | 391.19 | J/mol×K | 908.23 | 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=C6373155&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 |