# PHENYLFORMAMINIDE, N-ACETYL-

**Other names:** N-Acetylbenzamide
**Inchi:** InChI=1S/C9H9NO2/c1-7(11)10-9(12)8-5-3-2-4-6-8/h2-6H,1H3,(H,10,11,12)
**InchiKey:** KGGRQKDGRGUWAT-UHFFFAOYSA-N
**Formula:** C9H9NO2
**SMILES:** CC(=O)NC(=O)c1ccccc1
**Mol. weight [g/mol]:** 163.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5490 | | Cheméo Relay (1.0) |
| gf | -31.14 | kJ/mol | Joback Method |
| hf | -303.74 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 21.40 | kJ/mol | Joback Method |
| hvap | 72.29 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.14 | eV | Cheméo Relay (1.0) |
| log10ws | -1.60 | | Cheméo Relay (1.0) |
| logp | 0.963 | | Crippen Method |
| mcvol | 127.030 | ml/mol | McGowan Method |
| pc | 3848.31 | kPa | Joback Method |
| tb | 554.30 | K | Cheméo Relay (1.0) |
| tc | 789.35 | K | Cheméo Relay (1.0) |
| tf | 373.42 | K | Cheméo Relay (1.0) |
| vc | 0.459 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 292.82 | J/mol×K | 589.91 | Joback Method |
| cpg | 304.47 | J/mol×K | 627.73 | Joback Method |
| cpg | 315.28 | J/mol×K | 665.55 | Joback Method |
| cpg | 325.28 | J/mol×K | 703.37 | Joback Method |
| cpg | 334.51 | J/mol×K | 741.19 | Joback Method |
| cpg | 343.02 | J/mol×K | 779.02 | Joback Method |
| cpg | 350.83 | J/mol×K | 816.84 | Joback Method |

# Sources

| | |
|---|---|
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1575957&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **af:** | Acentric Factor |
| **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 |
| **ie:** | Ionization energy |
| **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 |