

# N-Acetyl-N-(4-methoxyphenyl)acetamide

|                      |                                                                        |
|----------------------|------------------------------------------------------------------------|
| Other names:         | 4-(Diacetylamino)anisole<br>N-(4-Methoxyphenyl)diacetamide             |
| Inchi:               | InChI=1S/C11H13NO3/c1-8(13)12(9(2)14)10-4-6-11(15-3)7-5-10/h4-7H,1-3H3 |
| InchiKey:            | NWBPJGXONLXNMX-UHFFFAOYSA-N                                            |
| Formula:             | C11H13NO3                                                              |
| SMILES:              | COc1ccc(N(C(C)=O)C(C)=O)cc1                                            |
| Mol. weight [g/mol]: | 207.23                                                                 |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -107.54 | kJ/mol  | Joback Method  |
| hf            | -335.16 | kJ/mol  | Joback Method  |
| hfus          | 25.30   | kJ/mol  | Joback Method  |
| hvap          | 60.96   | kJ/mol  | Joback Method  |
| log10ws       | -1.89   |         | Crippen Method |
| logp          | 1.595   |         | Crippen Method |
| mcvol         | 161.080 | ml/mol  | McGowan Method |
| pc            | 2918.68 | kPa     | Joback Method  |
| rinpol        | 1663.00 |         | NIST Webbook   |
| tb            | 625.34  | K       | Joback Method  |
| tc            | 840.07  | K       | Joback Method  |
| tf            | 407.23  | K       | Joback Method  |
| vc            | 0.592   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 399.16 | J/mol×K | 625.34          | Joback Method |
| cpg           | 412.52 | J/mol×K | 661.13          | Joback Method |
| cpg           | 425.03 | J/mol×K | 696.92          | Joback Method |
| cpg           | 436.70 | J/mol×K | 732.70          | Joback Method |
| cpg           | 447.56 | J/mol×K | 768.49          | Joback Method |
| cpg           | 457.64 | J/mol×K | 804.28          | Joback Method |
| cpg           | 466.95 | J/mol×K | 840.07          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U373212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373212&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvac:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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