

# Acetamide, N-(4-methoxyphenyl)-2-phenyl-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H15NO2/c1-18-14-9-7-13(8-10-14)16-15(17)11-12-5-3-2-4-6-12/h2-10H,11H,12H,14H,15H,16H,17H,18H

LZSPYXRRVCVACQ-UHFFFAOYSA-N

C15H15NO2

COc1ccc(NC(=O)Cc2ccccc2)cc1

241.29

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 146.08  | kJ/mol  | Joback Method  |
| hf            | -82.67  | kJ/mol  | Joback Method  |
| hfus          | 30.18   | kJ/mol  | Joback Method  |
| hvap          | 69.79   | kJ/mol  | Joback Method  |
| log10ws       | -3.41   |         | Crippen Method |
| logp          | 2.876   |         | Crippen Method |
| mcvol         | 192.110 | ml/mol  | McGowan Method |
| pc            | 2624.46 | kPa     | Joback Method  |
| rinpol        | 2224.00 |         | NIST Webbook   |
| rinpol        | 2224.00 |         | NIST Webbook   |
| tb            | 727.40  | K       | Joback Method  |
| tc            | 963.37  | K       | Joback Method  |
| tf            | 448.99  | K       | Joback Method  |
| vc            | 0.719   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 517.85 | J/mol×K | 727.40          | Joback Method |
| cpg           | 532.62 | J/mol×K | 766.73          | Joback Method |
| cpg           | 546.20 | J/mol×K | 806.06          | Joback Method |
| cpg           | 558.64 | J/mol×K | 845.39          | Joback Method |
| cpg           | 570.00 | J/mol×K | 884.72          | Joback Method |
| cpg           | 580.32 | J/mol×K | 924.05          | Joback Method |
| cpg           | 589.66 | J/mol×K | 963.37          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <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=U307144&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307144&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>                                 |

# 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>hvap:</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>rlnpol:</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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