

# Benzamide, N-tetrahydrofurfuryl-4-methoxy-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C13H17NO3/c1-16-11-6-4-10(5-7-11)13(15)14-9-12-3-2-8-17-12/h4-7,12H,2-3 |
| <b>InchiKey:</b>            | FGHCTPHRJXBK-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C13H17NO3  |
| <b>SMILES:</b>              | COc1ccc(C(=O)NCC2CCCO2)cc1   |
| <b>Mol. weight [g/mol]:</b> | 235.28   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -32.74  | kJ/mol               | Joback Method  |
| hf            | -349.44 | kJ/mol               | Joback Method  |
| hfus          | 32.88   | kJ/mol               | Joback Method  |
| hvap          | 67.83   | kJ/mol               | Joback Method  |
| log10ws       | -2.70   |                      | Crippen Method |
| logp          | 1.604   |                      | Crippen Method |
| mvol          | 182.700 | ml/mol               | McGowan Method |
| pc            | 2712.67 | kPa                  | Joback Method  |
| rinpol        | 2135.00 |                      | NIST Webbook   |
| rinpol        | 2135.00 |                      | NIST Webbook   |
| tb            | 697.19  | K                    | Joback Method  |
| tc            | 925.39  | K                    | Joback Method  |
| tf            | 437.50  | K                    | Joback Method  |
| vc            | 0.676   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 517.11 | J/molxK | 697.19          | Joback Method |
| cpg           | 533.36 | J/molxK | 735.22          | Joback Method |
| cpg           | 548.41 | J/molxK | 773.26          | Joback Method |
| cpg           | 562.32 | J/molxK | 811.29          | Joback Method |
| cpg           | 575.12 | J/molxK | 849.32          | Joback Method |
| cpg           | 586.84 | J/molxK | 887.35          | Joback Method |
| cpg           | 597.53 | J/molxK | 925.39          | 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=U307493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307493&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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