

# Benzamide, 4-methyl-N-butyl-N-dodecyl-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C24H41NO/c1-4-6-8-9-10-11-12-13-14-15-21-25(20-7-5-2)24(26)23-18-16-22( |
| <b>InchiKey:</b>            | KKKXCICKHGSNTEX-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C24H41NO   |
| <b>SMILES:</b>              | CCCCCCCCCCCCN(CCCC)C(=O)c1ccc(C)cc1  |
| <b>Mol. weight [g/mol]:</b> | 359.59   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 235.84  | kJ/mol               | Joback Method  |
| hf            | -358.68 | kJ/mol               | Joback Method  |
| hfus          | 56.19   | kJ/mol               | Joback Method  |
| hvap          | 80.75   | kJ/mol               | Joback Method  |
| log10ws       | -7.95   |                      | Crippen Method |
| logp          | 7.158   |                      | Crippen Method |
| mvol          | 336.810 | ml/mol               | McGowan Method |
| pc            | 1011.02 | kPa                  | Joback Method  |
| rinpol        | 1044.00 |                      | NIST Webbook   |
| rinpol        | 1044.00 |                      | NIST Webbook   |
| tb            | 846.49  | K                    | Joback Method  |
| tc            | 1040.82 | K                    | Joback Method  |
| tf            | 481.58  | K                    | Joback Method  |
| vc            | 1.296   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1079.35 | J/molxK | 846.49          | Joback Method |
| cpg           | 1099.01 | J/molxK | 878.88          | Joback Method |
| cpg           | 1117.54 | J/molxK | 911.27          | Joback Method |
| cpg           | 1135.00 | J/molxK | 943.66          | Joback Method |
| cpg           | 1151.44 | J/molxK | 976.04          | Joback Method |
| cpg           | 1166.94 | J/molxK | 1008.43         | Joback Method |
| cpg           | 1181.56 | J/molxK | 1040.82         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <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=U415929&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415929&amp;Units=SI</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>rinpola:</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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