

# Butanamide, N,N-dibutyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Butyramide, N,N-dibutyl-  |
| <b>Inchi:</b>               | InChI=1S/C12H25NO/c1-4-7-10-13(11-8-5-2)12(14)9-6-3/h4-11H2,1-3H3 |
| <b>InchiKey:</b>            | YIGDAUZYXKBHT-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C12H25NO  |
| <b>SMILES:</b>              | CCCCN(CCCC)C(=O)CCC   |
| <b>Mol. weight [g/mol]:</b> | 199.33  |
| <b>CAS:</b>                 | 14287-95-7  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 32.02   | kJ/mol  | Joback Method  |
| hf            | -336.06 | kJ/mol  | Joback Method  |
| hfus          | 31.46   | kJ/mol  | Joback Method  |
| hvap          | 51.09   | kJ/mol  | Joback Method  |
| log10ws       | -3.19   |         | Crippen Method |
| logp          | 3.215   |         | Crippen Method |
| mcvol         | 191.490 | ml/mol  | McGowan Method |
| pc            | 1875.65 | kPa     | Joback Method  |
| rinpol        | 1437.00 |         | NIST Webbook   |
| tb            | 540.27  | K       | Joback Method  |
| tc            | 709.01  | K       | Joback Method  |
| tf            | 307.40  | K       | Joback Method  |
| vc            | 0.732   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 472.67 | J/molxK | 540.27          | Joback Method |
| cpg           | 489.15 | J/molxK | 568.39          | Joback Method |
| cpg           | 504.91 | J/molxK | 596.52          | Joback Method |
| cpg           | 519.98 | J/molxK | 624.64          | Joback Method |
| cpg           | 534.38 | J/molxK | 652.77          | Joback Method |
| cpg           | 548.14 | J/molxK | 680.89          | Joback Method |
| cpg           | 561.27 | J/molxK | 709.01          | 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=C14287957&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14287957&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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