

# Pentanamide, N,N-dioctyl-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C21H43NO/c1-4-7-10-12-14-16-19-22(21(23)18-9-6-3)20-17-15-13-11-8-5-2/h |
| <b>InchiKey:</b>            | IIWWWQSXZQXFHJ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C21H43NO   |
| <b>SMILES:</b>              | CCCCCCCCN(CCCCCCCC)C(=O)CCCC   |
| <b>Mol. weight [g/mol]:</b> | 325.57   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 107.80  | kJ/mol               | Joback Method  |
| hf            | -521.82 | kJ/mol               | Joback Method  |
| hfus          | 54.77   | kJ/mol               | Joback Method  |
| hvap          | 71.13   | kJ/mol               | Joback Method  |
| log10ws       | -6.96   |                      | Crippen Method |
| logp          | 6.726   |                      | Crippen Method |
| mvol          | 318.300 | ml/mol               | McGowan Method |
| pc            | 993.25  | kPa                  | Joback Method  |
| rinpol        | 2313.00 |                      | NIST Webbook   |
| rinpol        | 2313.00 |                      | NIST Webbook   |
| tb            | 746.19  | K                    | Joback Method  |
| tc            | 918.15  | K                    | Joback Method  |
| tf            | 408.83  | K                    | Joback Method  |
| vc            | 1.236   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 979.39  | J/molxK | 746.19          | Joback Method |
| cpg           | 999.86  | J/molxK | 774.85          | Joback Method |
| cpg           | 1019.35 | J/molxK | 803.51          | Joback Method |
| cpg           | 1037.90 | J/molxK | 832.17          | Joback Method |
| cpg           | 1055.56 | J/molxK | 860.83          | Joback Method |
| cpg           | 1072.36 | J/molxK | 889.49          | Joback Method |
| cpg           | 1088.34 | J/molxK | 918.15          | 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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U308185&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308185&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>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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