

# 3-Piperidinecarboxamide, N,N-diethyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | N,N-Diethylnipecotamide<br>Nipecotamide, N,N-diethyl-<br>3-(N,N-Diethylcarbamoyl)piperidine<br>N,N-Diethylnipeotamide<br>N,N-diethylpiperidine-3-carboxamide |
| <b>Inchi:</b>               | InChI=1S/C10H20N2O/c1-3-12(4-2)10(13)9-6-5-7-11-8-9/h9,11H,3-8H2,1-2H3   |
| <b>InchiKey:</b>            | ZXQKYQVJDR TTLZ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C10H20N2O  |
| <b>SMILES:</b>              | CCN(CC)C(=O)C1CCCNC1   |
| <b>Mol. weight [g/mol]:</b> | 184.28   |
| <b>CAS:</b>                 | 3367-95-1  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 127.34  | kJ/mol               | Joback Method  |
| hf            | -202.65 | kJ/mol               | Joback Method  |
| hfus          | 27.70   | kJ/mol               | Joback Method  |
| hvap          | 53.83   | kJ/mol               | Joback Method  |
| log10ws       | -1.20   |                      | Crippen Method |
| logp          | 0.854   |                      | Crippen Method |
| mcvol         | 162.430 | ml/mol               | McGowan Method |
| pc            | 2808.38 | kPa                  | Joback Method  |
| tb            | 562.61  | K                    | Joback Method  |
| tc            | 771.81  | K                    | Joback Method  |
| tf            | 397.27  | K                    | Joback Method  |
| vc            | 0.590   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 412.79 | J/mol×K | 562.61          | Joback Method |
| cpg           | 431.49 | J/mol×K | 597.48          | Joback Method |
| cpg           | 449.14 | J/mol×K | 632.34          | Joback Method |
| cpg           | 465.77 | J/mol×K | 667.21          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 481.40 | J/mol×K | 702.07 | Joback Method |
| cpg | 496.07 | J/mol×K | 736.94 | Joback Method |
| cpg | 509.80 | J/mol×K | 771.81 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C3367951&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3367951&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>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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