

# N,N-Dipropylformamide

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Formamide, N,N-di-n-propyl-<br>Formamide, N,N-dipropyl-<br>N,N-di-n-Propylformamide<br>N-N-di-n-propylformamide |
| <b>Inchi:</b>               | InChI=1S/C7H15NO/c1-3-5-8(7-9)6-4-2/h7H,3-6H2,1-2H3   |
| <b>InchiKey:</b>            | XFTIKWYXFSNCQF-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C7H15NO   |
| <b>SMILES:</b>              | CCCN(C=O)CCC  |
| <b>Mol. weight [g/mol]:</b> | 129.20  |
| <b>CAS:</b>                 | 6282-00-4   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 19.32   | kJ/mol               | Joback Method  |
| hf            | -205.86 | kJ/mol               | Joback Method  |
| hfus          | 19.20   | kJ/mol               | Joback Method  |
| hvap          | 39.94   | kJ/mol               | Joback Method  |
| log10ws       | -1.10   |                      | Crippen Method |
| logp          | 1.265   |                      | Crippen Method |
| mcvol         | 121.040 | ml/mol               | McGowan Method |
| pc            | 3025.61 | kPa                  | Joback Method  |
| tb            | 420.66  | K                    | Joback Method  |
| tc            | 590.90  | K                    | Joback Method  |
| tf            | 243.12  | K                    | Joback Method  |
| vc            | 0.463   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 311.23 | J/mol×K | 590.90          | Joback Method |
| cpg           | 301.56 | J/mol×K | 562.53          | Joback Method |
| cpg           | 291.44 | J/mol×K | 534.15          | Joback Method |
| cpg           | 280.85 | J/mol×K | 505.78          | Joback Method |
| cpg           | 269.77 | J/mol×K | 477.41          | Joback Method |

|      |        |         |        |   |
|------|--------|---------|--------|---|
| cpg  | 258.20 | J/molxK | 449.03 | Joback Method   |
| cpg  | 246.12 | J/molxK | 420.66 | Joback Method   |
| pvap | 0.06   | kPa     | 308.20 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.02   | kPa     | 294.80 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.03   | kPa     | 298.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.04   | kPa     | 301.20 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.03   | kPa     | 299.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.02   | kPa     | 295.80 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.05   | kPa     | 305.10 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.05   | kPa     | 306.10 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.06   | kPa     | 307.20 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.03   | kPa     | 296.50 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.04   | kPa     | 302.90 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |

|      |          |     |        |   |
|------|----------|-----|--------|---|
| pvap | 0.08     | kPa | 310.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.08     | kPa | 311.30 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.09     | kPa | 313.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.11     | kPa | 315.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.11     | kPa | 316.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.15     | kPa | 319.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.13     | kPa | 318.50 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.02     | kPa | 292.20 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.02     | kPa | 290.20 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 0.01     | kPa | 288.20 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 8.14e-03 | kPa | 283.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 7.41e-03 | kPa | 282.40 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |

|      |          |     |        |   |
|------|----------|-----|--------|---|
| pvap | 9.49e-03 | kPa | 285.10 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |
| pvap | 5.16e-03 | kPa | 278.50 | Vapour pressures and enthalpies of vaporisation of alkyl formamides |

## Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 373.50 ± 0.50 | K    | 2.40           | NIST Webbook |

## 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>Vapour pressures and enthalpies of vaporisation of alkyl formamides:</b> | <a href="https://www.doi.org/10.1016/j.fluid.2019.04.036">https://www.doi.org/10.1016/j.fluid.2019.04.036</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=C6282004&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6282004&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>pvap:</b>    | Vapor pressure                                  |
| <b>tb:</b>      | Normal Boiling Point Temperature                |

|              |                                   |
|--------------|-----------------------------------|
| <b>tbrp:</b> | Boiling point at reduced pressure |
| <b>tc:</b>   | Critical Temperature              |
| <b>tf:</b>   | Normal melting (fusion) point     |
| <b>vc:</b>   | Critical Volume                   |

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