

# N-propylurea

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C4H10N2O/c1-2-3-6-4(5)7/h2-3H2,1H3,(H3,5,6,7) |
| <b>InchiKey:</b>            | ZQZJKHIIQFPZCS-UHFFFAOYSA-N                            |
| <b>Formula:</b>             | C4H10N2O   |
| <b>SMILES:</b>              | CCCNC(N)=O   |
| <b>Mol. weight [g/mol]:</b> | 102.14   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 9.72    | kJ/mol  | Joback Method  |
| hf            | -151.21 | kJ/mol  | Joback Method  |
| hfus          | 18.01   | kJ/mol  | Joback Method  |
| hvap          | 48.32   | kJ/mol  | Joback Method  |
| log10ws       | -0.87   |         | Crippen Method |
| logp          | 0.065   |         | Crippen Method |
| mcvol         | 88.750  | ml/mol  | McGowan Method |
| pc            | 4634.00 | kPa     | Joback Method  |
| tb            | 467.49  | K       | Joback Method  |
| tc            | 665.92  | K       | Joback Method  |
| tf            | 320.69  | K       | Joback Method  |
| vc            | 0.330   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 189.41 | J/molxK | 467.49          | Joback Method |
| cpg           | 198.33 | J/molxK | 500.56          | Joback Method |
| cpg           | 206.83 | J/molxK | 533.63          | Joback Method |
| cpg           | 214.91 | J/molxK | 566.71          | Joback Method |
| cpg           | 222.59 | J/molxK | 599.78          | Joback Method |
| cpg           | 229.88 | J/molxK | 632.85          | Joback Method |
| cpg           | 236.79 | J/molxK | 665.92          | Joback Method |

|      |          |     |        |  |
|------|----------|-----|--------|--|
| psub | 4.70e-04 | kPa | 342.20 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |
| psub | 3.00e-04 | kPa | 337.40 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |
| psub | 1.90e-04 | kPa | 333.20 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |
| psub | 7.20e-04 | kPa | 345.70 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |

|      |          |     |        |  |
|------|----------|-----|--------|--|
| psub | 7.40e-04 | kPa | 346.10 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |
| psub | 9.40e-04 | kPa | 348.70 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |
| psub | 9.90e-04 | kPa | 349.20 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |
| psub | 1.08e-03 | kPa | 350.20 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |

|      |          |     |        |  |
|------|----------|-----|--------|--|
| psub | 1.58e-03 | kPa | 354.10 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |
| psub | 1.76e-03 | kPa | 355.20 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |
| psub | 2.17e-03 | kPa | 357.30 | Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea |

## Sources

|  |   |
|--|---|
| <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>     |
| <b>Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea:</b> | <a href="https://www.doi.org/10.1021/je050230z">https://www.doi.org/10.1021/je050230z</a>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                 |
| <b>McCowan Method:</b>   | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>psub:</b>    | Sublimation 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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