

# Propanamide, 3-phenyl-N-ethyl-N-heptyl-

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C18H29NO/c1-3-5-6-7-11-16-19(4-2)18(20)15-14-17-12-9-8-10-13-17/h8-10,12 |
| <b>InchiKey:</b>            | MLHKVYAOJSCULK-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C18H29NO  |
| <b>SMILES:</b>              | CCCCCCCN(CC)C(=O)CCc1ccccc1   |
| <b>Mol. weight [g/mol]:</b> | 275.43  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 194.95  | kJ/mol               | Joback Method  |
| hf            | -223.37 | kJ/mol               | Joback Method  |
| hfus          | 41.04   | kJ/mol               | Joback Method  |
| hvap          | 66.73   | kJ/mol               | Joback Method  |
| log10ws       | -4.81   |                      | Crippen Method |
| logp          | 4.438   |                      | Crippen Method |
| mvol          | 252.270 | ml/mol               | McGowan Method |
| pc            | 1533.06 | kPa                  | Joback Method  |
| rinpol        | 2378.00 |                      | NIST Webbook   |
| rinpol        | 2378.00 |                      | NIST Webbook   |
| tb            | 704.23  | K                    | Joback Method  |
| tc            | 895.36  | K                    | Joback Method  |
| tf            | 401.44  | K                    | Joback Method  |
| vc            | 0.960   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 722.05 | J/mol×K | 704.23          | Joback Method |
| cpg           | 740.34 | J/mol×K | 736.09          | Joback Method |
| cpg           | 757.59 | J/mol×K | 767.94          | Joback Method |
| cpg           | 773.85 | J/mol×K | 799.80          | Joback Method |
| cpg           | 789.17 | J/mol×K | 831.65          | Joback Method |
| cpg           | 803.60 | J/mol×K | 863.51          | Joback Method |
| cpg           | 817.18 | J/mol×K | 895.36          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U415398&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415398&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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