

# 1-Methyldecylamine

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 2-Undecylamine<br>2-Undecanamine<br>2-Aminoundecane               |
| <b>Inchi:</b>               | InChI=1S/C11H25N/c1-3-4-5-6-7-8-9-10-11(2)12/h11H,3-10,12H2,1-2H3 |
| <b>InchiKey:</b>            | NHBKWZCTSMCKDS-UHFFFAOYSA-N                                       |
| <b>Formula:</b>             | C11H25N   |
| <b>SMILES:</b>              | CCCCCCCCC(C)N   |
| <b>Mol. weight [g/mol]:</b> | 171.32  |
| <b>CAS:</b>                 | 13205-56-6  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 105.75  | kJ/mol  | Joback Method  |
| hf            | -241.86 | kJ/mol  | Joback Method  |
| hfus          | 25.92   | kJ/mol  | Joback Method  |
| hvap          | 50.33   | kJ/mol  | Joback Method  |
| log10ws       | -3.97   |         | Crippen Method |
| logp          | 3.474   |         | Crippen Method |
| mcvol         | 175.830 | ml/mol  | McGowan Method |
| pc            | 2049.31 | kPa     | Joback Method  |
| tb            | 523.17  | K       | Joback Method  |
| tc            | 699.47  | K       | Joback Method  |
| tf            | 281.99  | K       | Joback Method  |
| vc            | 0.674   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 430.51 | J/molxK | 523.17          | Joback Method |
| cpg           | 447.00 | J/molxK | 552.55          | Joback Method |
| cpg           | 462.80 | J/molxK | 581.94          | Joback Method |
| cpg           | 477.92 | J/molxK | 611.32          | Joback Method |
| cpg           | 492.37 | J/molxK | 640.70          | Joback Method |
| cpg           | 506.19 | J/molxK | 670.09          | 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.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=C13205566&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13205566&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>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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