

# 1-HEPTADECANAMINE, N,N-DIMETHYL-

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | N,N-dimethylheptadecylamine                                                       |
| Inchi:               | InChI=1S/C19H41N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2)3/h4-19H2,1-3H |
| InchiKey:            | WCVHUIPWSPEOIG-UHFFFAOYSA-N                                                       |
| Formula:             | C19H41N                                                                           |
| SMILES:              | CCCCCCCCCCCCCCCCCN(C)C                                                            |
| Mol. weight [g/mol]: | 283.54                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.8362  |         | Cheméo Relay (1.0) |
| gf            | 219.88  | kJ/mol  | Joback Method      |
| hf            | -376.61 | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 47.99   | kJ/mol  | Joback Method      |
| hvap          | 94.67   | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 8.40    | eV      | Cheméo Relay (1.0) |
| log10ws       | -6.89   |         | Cheméo Relay (1.0) |
| logp          | 6.419   |         | Crippen Method     |
| mcvol         | 288.550 | ml/mol  | McGowan Method     |
| pc            | 1079.22 | kPa     | Joback Method      |
| tb            | 584.98  | K       | Cheméo Relay (1.0) |
| tc            | 747.71  | K       | Cheméo Relay (1.0) |
| tf            | 299.79  | K       | Cheméo Relay (1.0) |
| vc            | 1.159   | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 823.56 | J/mol×K | 646.56          | Joback Method |
| cpg           | 844.31 | J/mol×K | 673.13          | Joback Method |
| cpg           | 864.20 | J/mol×K | 699.70          | Joback Method |
| cpg           | 883.26 | J/mol×K | 726.28          | Joback Method |
| cpg           | 901.50 | J/mol×K | 752.85          | Joback Method |
| cpg           | 918.97 | J/mol×K | 779.42          | Joback Method |
| cpg           | 935.68 | J/mol×K | 805.99          | Joback Method |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3002571&Units=SI>

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Cheméo Relay (1.0):**

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <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>ie:</b>      | Ionization energy                               |
| <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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