

# Dibenzylamine, 4,4'-dimethyl-

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C16H19N/c1-13-3-7-15(8-4-13)11-17-12-16-9-5-14(2)6-10-16/h3-10,17H,11-12 |
| InchiKey:            | XKUYLMSRDBGFLFH-UHFFFAOYSA-N                                                      |
| Formula:             | C16H19N                                                                           |
| SMILES:              | Cc1ccc(CNCc2ccc(C)cc2)cc1                                                         |
| Mol. weight [g/mol]: | 225.33                                                                            |
| CAS:                 | 98180-43-9                                                                        |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 378.79  | kJ/mol  | Joback Method  |
| hf            | 130.02  | kJ/mol  | Joback Method  |
| hfus          | 29.60   | kJ/mol  | Joback Method  |
| hvap          | 63.52   | kJ/mol  | Joback Method  |
| log10ws       | -5.02   |         | Crippen Method |
| logp          | 3.593   |         | Crippen Method |
| mcvol         | 198.760 | ml/mol  | McGowan Method |
| pc            | 2248.26 | kPa     | Joback Method  |
| tb            | 678.97  | K       | Joback Method  |
| tc            | 908.92  | K       | Joback Method  |
| tf            | 400.62  | K       | Joback Method  |
| vc            | 0.750   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 526.47 | J/mol×K | 678.97          | Joback Method |
| cpg           | 543.82 | J/mol×K | 717.30          | Joback Method |
| cpg           | 559.95 | J/mol×K | 755.62          | Joback Method |
| cpg           | 574.94 | J/mol×K | 793.95          | Joback Method |
| cpg           | 588.84 | J/mol×K | 832.27          | Joback Method |
| cpg           | 601.72 | J/mol×K | 870.60          | Joback Method |
| cpg           | 613.65 | J/mol×K | 908.92          | 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=C98180439&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C98180439&amp;Units=SI</a> |
| <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>                                     |

## 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>hvac:</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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