

# 1,6-Hexanediamine, N,N,N',N'-tetramethyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | (CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>6</sub> N(CH <sub>3</sub> ) <sub>2</sub><br>1,6-Bis(dimethylamino)hexane<br>Hexamethylenebis(dimethylamine)<br>N,N,N',N'-Tetramethyl-1,6-diaminohexane<br>N,N,N',N'-Tetramethyl-1,6-hexanediamine<br>N,N,N',N'-Tetramethylhexamethylenediamine |
| <b>Inchi:</b>               | InChI=1S/C10H24N2/c1-11(2)9-7-5-6-8-10-12(3)4/h5-10H2,1-4H3   |
| <b>InchiKey:</b>            | TXXWBTOATXBWDR-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C <sub>10</sub> H <sub>24</sub> N <sub>2</sub>  |
| <b>SMILES:</b>              | CN(C)CCCCCN(C)C   |
| <b>Mol. weight [g/mol]:</b> | 172.31  |
| <b>CAS:</b>                 | 111-18-2  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| affp          | 1035.80 | kJ/mol               | NIST Webbook   |
| basg          | 982.20  | kJ/mol               | NIST Webbook   |
| gf            | 254.88  | kJ/mol               | Joback Method  |
| hf            | -114.67 | kJ/mol               | Joback Method  |
| hfus          | 27.70   | kJ/mol               | Joback Method  |
| hvap          | 41.94   | kJ/mol               | Joback Method  |
| log10ws       | -1.15   |                      | Crippen Method |
| logp          | 1.670   |                      | Crippen Method |
| mcvol         | 171.720 | ml/mol               | McGowan Method |
| pc            | 2100.34 | kPa                  | Joback Method  |
| tb            | 482.70  | K                    | NIST Webbook   |
| tc            | 613.08  | K                    | Joback Method  |
| tf            | 267.40  | K                    | Joback Method  |
| vc            | 0.631   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 380.84 | J/mol×K | 453.08          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 397.52 | J/mol×K | 479.75 | Joback Method |
| cpg | 413.52 | J/mol×K | 506.41 | Joback Method |
| cpg | 428.85 | J/mol×K | 533.08 | Joback Method |
| cpg | 443.53 | J/mol×K | 559.75 | Joback Method |
| cpg | 457.59 | J/mol×K | 586.41 | Joback Method |
| cpg | 471.05 | J/mol×K | 613.08 | Joback Method |

## Sources

|  |   |
|--|---|
| <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=C111182&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C111182&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>                                 |
| <b>Crippen Method:</b>   | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>CO2 Solubility Measurements and Modeling for Tertiary Diamines:</b> | <a href="https://www.doi.org/10.1021/je500927h">https://www.doi.org/10.1021/je500927h</a>   |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|                 |   |
|-----------------|---|
| <b>affp:</b>    | Proton affinity                                 |
| <b>basg:</b>    | Gas basicity                                    |
| <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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