

# 1,2-Benzenediamine, N,N,N'-trimethyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 1,2-Phenylenediamine, N,N,N'-trimethyl-                    |
| <b>Inchi:</b>               | InChI=1S/C9H14N2/c1-10-8-6-4-5-7-9(8)11(2)3/h4-7,10H,1-3H3 |
| <b>InchiKey:</b>            | BXBFTMKSQSKHMF-UHFFFAOYSA-N                                |
| <b>Formula:</b>             | C9H14N2  |
| <b>SMILES:</b>              | CNc1ccccc1N(C)C  |
| <b>Mol. weight [g/mol]:</b> | 150.22   |
| <b>CAS:</b>                 | 2427-03-4  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 327.85  | kJ/mol  | Joback Method  |
| hf            | 116.97  | kJ/mol  | Joback Method  |
| hfus          | 20.84   | kJ/mol  | Joback Method  |
| hvap          | 47.05   | kJ/mol  | Joback Method  |
| log10ws       | -1.39   |         | Crippen Method |
| logp          | 1.794   |         | Crippen Method |
| mcvol         | 133.870 | ml/mol  | McGowan Method |
| pc            | 3246.73 | kPa     | Joback Method  |
| rinpol        | 1279.00 |         | NIST Webbook   |
| tb            | 499.59  | K       | Joback Method  |
| tc            | 707.32  | K       | Joback Method  |
| tf            | 315.26  | K       | Joback Method  |
| vc            | 0.484   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 293.56 | J/molxK | 499.59          | Joback Method |
| cpg           | 308.28 | J/molxK | 534.21          | Joback Method |
| cpg           | 322.14 | J/molxK | 568.83          | Joback Method |
| cpg           | 335.17 | J/molxK | 603.45          | Joback Method |
| cpg           | 347.41 | J/molxK | 638.07          | Joback Method |
| cpg           | 358.90 | J/molxK | 672.70          | Joback Method |
| cpg           | 369.67 | J/molxK | 707.32          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2427034&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2427034&amp;Units=SI</a> |
| <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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>                       |

# 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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