

# 1,2-Cyclobutane, bis-(methylamine)-

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C6H14N2/c7-3-5-1-2-6(5)4-8/h5-6H,1-4,7-8H2 |
| <b>InchiKey:</b>            | ZBLACDIKXKCJGF-UHFFFAOYSA-N                         |
| <b>Formula:</b>             | C6H14N2   |
| <b>SMILES:</b>              | NCC1CCC1CN  |
| <b>Mol. weight [g/mol]:</b> | 114.19  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 173.48  | kJ/mol  | Joback Method  |
| hf            | -53.29  | kJ/mol  | Joback Method  |
| hfus          | 18.80   | kJ/mol  | Joback Method  |
| hvap          | 50.01   | kJ/mol  | Joback Method  |
| log10ws       | -0.61   |         | Crippen Method |
| logp          | -0.070  |         | Crippen Method |
| mcvol         | 104.500 | ml/mol  | McGowan Method |
| pc            | 4119.70 | kPa     | Joback Method  |
| tb            | 488.08  | K       | Joback Method  |
| tc            | 704.18  | K       | Joback Method  |
| tf            | 334.08  | K       | Joback Method  |
| vc            | 0.378   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 250.89 | J/molxK | 488.08          | Joback Method |
| cpg           | 265.05 | J/molxK | 524.10          | Joback Method |
| cpg           | 278.40 | J/molxK | 560.11          | Joback Method |
| cpg           | 290.97 | J/molxK | 596.13          | Joback Method |
| cpg           | 302.80 | J/molxK | 632.15          | Joback Method |
| cpg           | 313.92 | J/molxK | 668.17          | Joback Method |
| cpg           | 324.36 | J/molxK | 704.18          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=B6006704&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6006704&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>mccvol:</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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