

# Pyrrolidine, 2,5-dimethyl-

|                      |                                                    |
|----------------------|----------------------------------------------------|
| Other names:         | Pyrrolidine, 2,5-dimethyl-                         |
| Inchi:               | InChI=1S/C6H13N/c1-5-3-4-6(2)7-5/h5-7H,3-4H2,1-2H3 |
| InchiKey:            | ZEBFPAXSQXIPNF-UHFFFAOYSA-N                        |
| Formula:             | C6H13N                                             |
| SMILES:              | CC1CCC(C)N1                                        |
| Mol. weight [g/mol]: | 99.18                                              |

## Physical Properties

| Property code | Value  | Unit   | Source             |
|---------------|--------|--------|--------------------|
| hf            | -88.81 | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 15.89  | kJ/mol | Joback Method      |
| hvap          | 36.51  | kJ/mol | Cheméo Relay (1.0) |
| ie            | 7.84   | eV     | Cheméo Relay (1.0) |
| logp          | 1.147  |        | Crippen Method     |
| mcvol         | 94.520 | ml/mol | McGowan Method     |
| rinpol        | 756.00 |        | NIST Webbook       |
| rinpol        | 756.00 |        | NIST Webbook       |
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| tb            | 378.22 | K      | Cheméo Relay (1.0) |
| tc            | 575.43 | K      | Cheméo Relay (1.0) |
| tf            | 233.44 | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 176.49 | J/mol×K | 395.84          | Joback Method |
| cpg           | 191.02 | J/mol×K | 429.94          | Joback Method |
| cpg           | 204.93 | J/mol×K | 464.03          | Joback Method |
| cpg           | 218.24 | J/mol×K | 498.13          | Joback Method |
| cpg           | 230.95 | J/mol×K | 532.22          | Joback Method |
| cpg           | 243.08 | J/mol×K | 566.32          | Joback Method |
| cpg           | 254.63 | J/mol×K | 600.42          | Joback Method |

# Sources

|                                  |                                                                                                                                             |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3378710&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3378710&amp;Units=SI</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>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>Cheméo Relay (1.0):</b>       |                                                                                                                                             |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                             |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>rinpola:</b> | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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