

# Piperidine, 1,2-dimethyl-

|                             |                                                    |
|-----------------------------|----------------------------------------------------|
| <b>Other names:</b>         | 1,2-Dimethylpiperidine                             |
| <b>Inchi:</b>               | InChI=1S/C7H15N/c1-7-5-3-4-6-8(7)2/h7H,3-6H2,1-2H3 |
| <b>InchiKey:</b>            | MWUISCCBFHLWLY-UHFFFAOYSA-N                        |
| <b>Formula:</b>             | C7H15N                                             |
| <b>SMILES:</b>              | CC1CCCCN1C                                         |
| <b>Mol. weight [g/mol]:</b> | 113.20                                             |
| <b>CAS:</b>                 | 671-36-3                                           |

## Physical Properties

| Property code | Value         | Unit   | Source         |
|---------------|---------------|--------|----------------|
| ie            | 7.63 ± 0.05   | eV     | NIST Webbook   |
| log10ws       | -1.33         |        | Crippen Method |
| logp          | 1.491         |        | Crippen Method |
| mcvol         | 108.610       | ml/mol | McGowan Method |
| rinpol        | 841.00        |        | NIST Webbook   |
| rinpol        | 834.00        |        | NIST Webbook   |
| ripol         | 1000.00       |        | NIST Webbook   |
| ripol         | 1000.00       |        | NIST Webbook   |
| tb            | 401.00 ± 1.00 | K      | NIST Webbook   |

## 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=C671363&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C671363&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>                         |

## Legend

|                 |                                    |
|-----------------|------------------------------------|
| <b>ie:</b>      | Ionization energy                  |
| <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>rinpol:</b> | Non-polar retention indices         |
| <b>ripol:</b>  | Polar retention indices             |
| <b>tb:</b>     | Normal Boiling Point Temperature    |

Latest version available from:

<https://www.cheméo.com/cid/21-484-1/Piperidine-1-2-dimethyl.pdf>

Generated by Cheméo on 2024-04-23 08:23:58.324172095 +0000 UTC m=+16149887.244749411.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.