

# Piperidine, 1,2,2,6,6-pentamethyl-

|                      |                                                                                                                                        |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1,2,2,6,6-Pentamethylpiperidine<br>M&B 4486<br>M+B 4486<br>N-Methyl-2,2,6,6-Tetramethylpiperidine<br>Perolysen<br>Pyrilene<br>Tenormal |
| Inchi:               | InChI=1S/C10H21N/c1-9(2)7-6-8-10(3,4)11(9)5/h6-8H2,1-5H3                                                                               |
| InchiKey:            | XULIXFLCVXWHRF-UHFFFAOYSA-N                                                                                                            |
| Formula:             | C10H21N                                                                                                                                |
| SMILES:              | CN1C(C)(C)CCCC1(C)C                                                                                                                    |
| Mol. weight [g/mol]: | 155.29                                                                                                                                 |
| CAS:                 | 79-55-0                                                                                                                                |

## Physical Properties

| Property code | Value       | Unit   | Source         |
|---------------|-------------|--------|----------------|
| ie            | 7.23 ± 0.05 | eV     | NIST Webbook   |
| logp          | 2.659       |        | Crippen Method |
| mcvol         | 150.880     | ml/mol | McGowan Method |
| tb            | 460.70      | K      | NIST Webbook   |
| tb            | 420.20      | K      | NIST Webbook   |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.17565e+01                   |
| Coeff. B                    | -2.87490e+03                  |
| Coeff. C                    | -5.79520e+01                  |
| Temperature range (K), min. | 308.62                        |
| Temperature range (K), max. | 504.01                        |

# 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>Cheméo Relay (1.0):</b>                  |                                                                                                                                                                                         |
| <b>Cheméo Relay (1.0, beta):</b>            |                                                                                                                                                                                         |
| <b>The Yaws Handbook of Vapor Pressure:</b> | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| <b>NIST Webbook:</b>                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C79550&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C79550&amp;Units=SI</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>ie:</b>    | Ionization energy                   |
| <b>logp:</b>  | Octanol/Water partition coefficient |
| <b>mcvol:</b> | McGowan's characteristic volume     |
| <b>pvap:</b>  | Vapor pressure                      |
| <b>tb:</b>    | Normal Boiling Point Temperature    |

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