

# 1H-Imidazole, 1,2-dimethyl-

|                      |                                                                                                                                |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1,2-dimethyl-1H-imidazole<br>1,2-dimethylimidazole<br>N,2-Dimethylimidazole<br>NSC 111174<br>SN 25<br>imidazole, 1,2-dimethyl- |
| Inchi:               | InChI=1S/C5H8N2/c1-5-6-3-4-7(5)2/h3-4H,1-2H3                                                                                   |
| InchiKey:            | GIWQSPITLQVMSG-UHFFFAOYSA-N                                                                                                    |
| Formula:             | C5H8N2                                                                                                                         |
| SMILES:              | Cc1nccn1C                                                                                                                      |
| Mol. weight [g/mol]: | 96.13                                                                                                                          |
| CAS:                 | 1739-84-0                                                                                                                      |

## Physical Properties

| Property code | Value   | Unit   | Source                             |
|---------------|---------|--------|------------------------------------|
| affp          | 984.70  | kJ/mol | NIST Webbook                       |
| basg          | 952.60  | kJ/mol | NIST Webbook                       |
| ie            | 8.38    | eV     | NIST Webbook                       |
| log10ws       | -3.00   |        | Crippen Method                     |
| logp          | 0.729   |        | Crippen Method                     |
| mcvol         | 81.810  | ml/mol | McGowan Method                     |
| rinpol        | 1006.00 |        | NIST Webbook                       |
| rinpol        | 1006.00 |        | NIST Webbook                       |
| rinpol        | 1006.00 |        | NIST Webbook                       |
| ripol         | 1715.00 |        | NIST Webbook                       |
| tb            | 479.20  | K      | NIST Webbook                       |
| tb            | 477.20  | K      | NIST Webbook                       |
| tf            | 311.50  | K      | Solubility of Imidazoles in Ethers |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1739840&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1739840&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Solubility of Imidazoles in Ethers:** <https://www.doi.org/10.1021/je020113t>  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>affp:</b>    | Proton affinity                     |
| <b>basg:</b>    | Gas basicity                        |
| <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    |
| <b>tf:</b>      | Normal melting (fusion) point       |

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