

# 4,5-DIPHENYLIMIDAZOLE

|                      |                                                                                                          |
|----------------------|----------------------------------------------------------------------------------------------------------|
| Other names:         | 4,5-Diphenylglyoxaline<br>4,5-diphenyl-1H-imidazole<br>4.5-Diphenylimidazole<br>Imidazole, 4,5-diphenyl- |
| Inchi:               | InChI=1S/C15H12N2/c1-3-7-12(8-4-1)14-15(17-11-16-14)13-9-5-2-6-10-13/h1-11H,(H,16)                       |
| InchiKey:            | CPHGOBGXZQKCKI-UHFFFAOYSA-N                                                                              |
| Formula:             | C15H12N2                                                                                                 |
| SMILES:              | c1ccc(-c2nc[nH]c2-c2ccccc2)cc1                                                                           |
| Mol. weight [g/mol]: | 220.28                                                                                                   |

## Physical Properties

| Property code | Value   | Unit   | Source                                                                                                                         |
|---------------|---------|--------|--------------------------------------------------------------------------------------------------------------------------------|
| hfus          | 34.19   | kJ/mol | Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene |
| logp          | 3.262   |        | Crippen Method                                                                                                                 |
| mcvol         | 175.190 | ml/mol | McGowan Method                                                                                                                 |

## Sources

|                                                                                                                                 |                                                                                                                                           |
|---------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| 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:                                                                                                                 | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Cheméo Relay (1.0):                                                                                                             |                                                                                                                                           |
| Cheméo Relay (1.0, beta):                                                                                                       |                                                                                                                                           |
| Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene: | <a href="https://www.doi.org/10.1021/je049907t">https://www.doi.org/10.1021/je049907t</a>                                                 |
| NIST Webbook:                                                                                                                   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C668940&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C668940&amp;Units=SI</a> |
| McGowan Method:                                                                                                                 | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |

## Legend

|               |                                           |
|---------------|-------------------------------------------|
| <b>hfus:</b>  | Enthalpy of fusion at standard conditions |
| <b>logp:</b>  | Octanol/Water partition coefficient       |
| <b>mcvol:</b> | McGowan's characteristic volume           |

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