

# 1,6-Naphthyridine

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 1,6-Diazanaphthalene<br>1,6-Pyridopyridine      |
| <b>Inchi:</b>               | InChI=1S/C8H6N2/c1-2-7-6-9-5-3-8(7)10-4-1/h1-6H |
| <b>InchiKey:</b>            | VSOSXKMEQPYESP-UHFFFAOYSA-N                     |
| <b>Formula:</b>             | C8H6N2  |
| <b>SMILES:</b>              | c1cnc2ccncc2c1                                  |
| <b>Mol. weight [g/mol]:</b> | 130.15  |
| <b>CAS:</b>                 | 253-72-5  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| ie            | 9.00    | eV     | NIST Webbook   |
| ie            | 9.07    | eV     | NIST Webbook   |
| log10ws       | -2.81   |        | Crippen Method |
| logp          | 1.630   |        | Crippen Method |
| mcvol         | 100.320 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C253725&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C253725&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>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>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |

Latest version available from:

<https://www.cheméo.com/cid/47-795-8/1-6-Naphthyridine.pdf>

Generated by Cheméo on 2024-04-19 18:22:51.226863495 +0000 UTC m=+15840220.147440810.

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