

# Pyridoxamine

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 3-Pyridinemethanol, 4-(aminomethyl)-5-hydroxy-6-methyl-Pyridoxylamine<br>3-Pyridinol, 2-methyl-4-aminomethyl-5-hydroxymethyl- |
| <b>Inchi:</b>               | InChI=1S/C8H12N2O2/c1-5-8(12)7(2-9)6(4-11)3-10-5/h3,11-12H,2,4,9H2,1H3  |
| <b>InchiKey:</b>            | NHZMQXZHNVTQA-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C8H12N2O2   |
| <b>SMILES:</b>              | <chem>Cc1ncc(CO)c(CN)c1O</chem>   |
| <b>Mol. weight [g/mol]:</b> | 168.19  |
| <b>CAS:</b>                 | 85-87-0   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -1.72   |        | Crippen Method |
| logp          | 0.047   |        | Crippen Method |
| mcvol         | 131.520 | ml/mol | McGowan Method |
| rinpol        | 2000.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <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>                   |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C85870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85870&amp;Units=SI</a> |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <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         |

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