

# 2-Pyridinamine, 3-nitro-

|                             |                                                                                                                                          |
|-----------------------------|------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Other names:</b>         | Pyridine, 2-amino-3-nitro-<br>2-Amino-3-nitropyridine<br>3-Nitro-2-amino pyridine<br>3-Nitro-2-pyridinamine<br>3-Nitro-pyridin-2-ylamine |
| <b>Inchi:</b>               | InChI=1S/C5H5N3O2/c6-5-4(8(9)10)2-1-3-7-5/h1-3H,(H2,6,7)                                                                                 |
| <b>InchiKey:</b>            | BPYHGTCRXDWOIQ-UHFFFAOYSA-N                                                                                                              |
| <b>Formula:</b>             | C5H5N3O2                                                                                                                                 |
| <b>SMILES:</b>              | <chem>Nc1cccc1[N+](=O)[O-]</chem>                                                                                                        |
| <b>Mol. weight [g/mol]:</b> | 139.11                                                                                                                                   |
| <b>CAS:</b>                 | 4214-75-9                                                                                                                                |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| log10ws       | -1.52  |        | Crippen Method |
| logp          | 0.572  |        | Crippen Method |
| mccvol        | 94.930 | ml/mol | McGowan Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=C4214759&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4214759&amp;Units=SI</a> |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mccvol:</b>  | McGowan's characteristic volume     |

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