

# 2(1H)-Pyridinone, 5-nitro-

|                      |                                                                                                                                                                                                                                    |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 5-Nitro-2-hydroxypyridine<br>5-Nitro-2-pyridinol<br>5-Nitro-2-pyridinone<br>5-Nitro-2(1H)-pyridinone<br>5-Nitro-2-pyridone<br>5-Nitro-2(1H)-pyridone<br>2-Pyridinol, 5-nitro-<br>2(1H)-Pyridinone, 5-nitro-<br>5-nitropyridin-2-ol |
| Inchi:               | InChI=1S/C5H4N2O3/c8-5-2-1-4(3-6-5)7(9)10/h1-3H,(H,6,8)                                                                                                                                                                            |
| InchiKey:            | XKWSQIMYNVLGBO-UHFFFAOYSA-N                                                                                                                                                                                                        |
| Formula:             | C5H4N2O3                                                                                                                                                                                                                           |
| SMILES:              | O=c1ccc([N+](=O)[O-])c[nH]1                                                                                                                                                                                                        |
| Mol. weight [g/mol]: | 140.10                                                                                                                                                                                                                             |

## Physical Properties

| Property code | Value  | Unit   | Source             |
|---------------|--------|--------|--------------------|
| hf            | -53.22 | kJ/mol | Cheméo Relay (1.0) |
| hvap          | 99.31  | kJ/mol | Cheméo Relay (1.0) |
| ie            | 9.81   | eV     | Cheméo Relay (1.0) |
| log10ws       | -1.20  |        | Cheméo Relay (1.0) |
| logp          | -0.199 |        | Crippen Method     |
| mcvol         | 90.820 | ml/mol | McGowan Method     |
| tb            | 563.67 | K      | Cheméo Relay (1.0) |
| tf            | 451.81 | K      | Cheméo Relay (1.0) |

## Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5418519&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

# Legend

|                            |                                                 |
|----------------------------|-------------------------------------------------|
| <b>hf:</b>                 | Enthalpy of formation at standard conditions    |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>                 | Ionization energy                               |
| <b>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>              | McGowan's characteristic volume                 |
| <b>tb:</b>                 | Normal Boiling Point Temperature                |
| <b>tf:</b>                 | Normal melting (fusion) point                   |

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