

# 4-AMINO-6-HYDROXY-2-METHYL-5-NITROSOPYRIMIDINE

|                      |                                                                                                                                                                                                  |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 4-Amino-6-hydroxy-2-methyl-5-nitrosopyrimidine<br>4-Pyrimidinol, 6-amino-2-methyl-5-nitroso-<br>4(3H)-Pyrimidinone, 6-amino-2-methyl-5-nitroso-<br>6-amino-2-methyl-5-nitroso-1H-pyrimidin-4-one |
| Inchi:               | InChI=1S/C5H6N4O2/c1-2-7-4(6)3(9-11)5(10)8-2/h1H3,(H3,6,7,8,10)                                                                                                                                  |
| InchiKey:            | DRDJDNORXOOBHR-UHFFFAOYSA-N                                                                                                                                                                      |
| Formula:             | C5H6N4O2                                                                                                                                                                                         |
| SMILES:              | Cc1nc(N)c(N=O)c(O)n1                                                                                                                                                                             |
| Mol. weight [g/mol]: | 154.13                                                                                                                                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| logp          | 0.471   |        | Crippen Method |
| mcvol         | 104.910 | ml/mol | McGowan Method |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| 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): |                                                                                                                                             |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2209725&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2209725&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>                       |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |

## Legend

|        |                                     |
|--------|-------------------------------------|
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |

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