# AMETAZOLE

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|---|---|
| **Other names:** | 1H-Pyrazole-3-ethanamine |
| | 3-(2-Aminoethyl)pyrazole |
| | 3-Aminoethylpyrazole |
| | Ametazole |
| | Pyrazole, 3-(2-aminoethyl)- |
| **Inchi:** | InChI=1S/C5H9N3/c6-3-1-5-2-4-7-8-5/h2,4H,1,3,6H2,(H,7,8) |
| **InchiKey:** | JXDFEQONERDKSS-UHFFFAOYSA-N |
| **Formula:** | C5H9N3 |
| **SMILES:** | NCCc1cc[nH]n1 |
| **Mol. weight [g/mol]:** | 111.15 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| logp | -0.571 | | Crippen Method |
| mcvol | 91.790 | ml/mol | McGowan Method |
| rinpol | 1390.00 | | NIST Webbook |

## Sources

| | |
|---|---|
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C105204&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

## Legend

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|---|---|
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |