# 6-Azauracil

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|---|---|
| **Other names:** | 1,2,4-triazine-3,5(2H,4H)-dione |
| | 1,2,4-triazine-3,5-diol |
| | 2,3,4,5-tetrahydro-1,2,4-triazine-3,5-dione |
| | 4(6)-Azauracil |
| | AZU |
| | Azauracil |
| | IPO 3834 |
| | NSC 3425 |
| | USAF CB-30 |
| | as-Triazine-3,5(2H,4H)-dione |
| | as-Triazine-3,5-diol |
| **Inchi:** | InChI=1S/C3H3N3O2/c7-2-1-4-6-3(8)5-2/h1H,(H2,5,6,7,8) |
| **InchiKey:** | SSPYSWLZOPCOLO-UHFFFAOYSA-N |
| **Formula:** | C3H3N3O2 |
| **SMILES:** | O=c1cn[nH]c(=O)[nH]1 |
| **Mol. weight [g/mol]:** | 113.08 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 10.00 | eV | NIST Webbook |
| ie | 10.20 ± 0.10 | eV | NIST Webbook |
| ie | 10.18 | eV | NIST Webbook |
| logp | -2.506 | | Crippen Method |
| mcvol | 71.050 | ml/mol | McGowan Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| hvapt | 118.10 | kJ/mol | 298.15 | Experimental and computational thermochemical studies of 6-azauracil derivatives |

# Sources

| | |
|---|---|
| **Cheméo Relay (1.0, beta):** | |
| **Experimental and computational thermochemical studies of 6-azauracil derivatives:** | https://www.doi.org/10.1016/j.jct.2015.12.020 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C461892&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 |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |