# 6H-Purin-6-one, 1,7-dihydro-1-methyl-

| | |
|---|---|
| **Other names:** | Hypoxanthine, 1-methyl-<br>1-Methylhypoxanthine<br>Purin-6(1H)-one, 1-methyl |
| **Inchi:** | InChI=1S/C6H6N4O/c1-10-3-9-5-4(6(10)11)7-2-8-5/h2-3H,1H3,(H,7,8) |
| **InchiKey:** | KIQMCGMHGVXDFW-UHFFFAOYSA-N |
| **Formula:** | C6H6N4O |
| **SMILES:** | Cn1cnc2[nH]cnc2c1=O |
| **Mol. weight [g/mol]:** | 150.14 |
| **CAS:** | 1125-39-9 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.74 | | Crippen Method |
| logp | -0.825 | | Crippen Method |
| mcvol | 102.270 | ml/mol | McGowan Method |
| rinpol | 1969.00 | | NIST Webbook |

## Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1125399&Units=SI |

## Legend

| | |
|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |

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