# 9H-Purin-6-amine,N,9-dimethyl-

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|---|---|
| **Other names:** | 6-Methylamino-9-methyl purine |
| **Inchi:** | InChI=1S/C7H9N5/c1-8-6-5-7(10-3-9-6)12(2)4-11-5/h3-4H,1-2H3,(H,8,9,10) |
| **InchiKey:** | GRDLXXJSRHDATN-UHFFFAOYSA-N |
| **Formula:** | C7H9N5 |
| **SMILES:** | CNc1ncnc2c1ncn2C |
| **Mol. weight [g/mol]:** | 163.18 |
| **CAS:** | 2009-52-1 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 7.95 | eV | NIST Webbook |
| log10ws | -3.87 | | Crippen Method |
| logp | 0.405 | | Crippen Method |
| mcvol | 120.470 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| hsubt | 115.50 ± 1.70 | kJ/mol | 352.50 | NIST Webbook |

## Sources

| | |
|---|---|
| **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=C2009521&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |

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