# 6-METHYLAMINO-9-METHYL PURINE

**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

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 7.95 | eV | NIST Webbook |
| 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

**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2009521&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

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