# 1H-Tetrazole, 1-methyl-

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|---|---|
| **Other names:** | N-Methyltetrazole |
| | 1-Methyl-1H-tetrazole |
| | 1-Methyltetrazole |
| **Inchi:** | InChI=1S/C2H4N4/c1-6-2-3-4-5-6/h2H,1H3 |
| **InchiKey:** | OMAFFHIGWTVZOH-UHFFFAOYSA-N |
| **Formula:** | C2H4N4 |
| **SMILES:** | Cn1cnnn1 |
| **Mol. weight [g/mol]:** | 84.08 |
| **CAS:** | 16681-77-9 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -1593.40 ± 0.40 | kJ/mol | NIST Webbook |
| hf | 322.90 ± 2.00 | kJ/mol | NIST Webbook |
| hfs | 234.70 ± 0.50 | kJ/mol | NIST Webbook |
| hsub | 88.20 ± 1.90 | kJ/mol | NIST Webbook |
| hsub | 88.20 | kJ/mol | NIST Webbook |
| ie | 10.30 | eV | NIST Webbook |
| log10ws | -2.06 | | Crippen Method |
| logp | -0.790 | | Crippen Method |
| mcvol | 59.500 | ml/mol | McGowan Method |
| tt | 315.00 ± 1.00 | K | NIST Webbook |
| tt | 316.00 ± 1.00 | K | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| hfust | 15.70 | kJ/mol | 315.00 | NIST Webbook |
| hfust | 15.70 | kJ/mol | 315.00 | NIST Webbook |
| hsubt | 86.70 ± 1.90 | kJ/mol | 296.50 | 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=C16681779&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **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 |
| **tt:** | Triple Point Temperature |