

1H-Tetrazole, 5-methyl-

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|-----------------------------|---|
| Other names: | 5-Methyltetrazole 2H-Tetrazole, 5-methyl- 5-Methyl-1H-tetrazole |
| Inchi: | InChI=1S/C2H4N4/c1-2-3-5-6-4-2/h1H3,(H,3,4,5,6) |
| InchiKey: | XZGLNCKSNVGDNX-UHFFFAOYSA-N |
| Formula: | C2H4N4 |
| SMILES: | Cc1nnn[nH]1 |
| Mol. weight [g/mol]: | 84.08 |
| CAS: | 4076-36-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|--------|----------------|
| chs | -1543.10 ± 2.50 | kJ/mol | NIST Webbook |
| hf | 280.70 ± 2.60 | kJ/mol | NIST Webbook |
| hfs | 184.40 ± 2.60 | kJ/mol | NIST Webbook |
| hsub | 96.30 ± 0.50 | kJ/mol | NIST Webbook |
| hsub | 96.30 | kJ/mol | NIST Webbook |
| log10ws | -0.46 | | Crippen Method |
| logp | -0.974 | | Crippen Method |
| mcvol | 59.500 | ml/mol | McGowan Method |
| tt | 418.00 ± 1.00 | K | NIST Webbook |
| tt | 420.00 ± 1.00 | K | NIST Webbook |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------------|--------|-----------------|--------------|
| hfust | 16.00 | kJ/mol | 418.00 | NIST Webbook |
| hfust | 16.00 | kJ/mol | 418.00 | NIST Webbook |
| hsubt | 93.80 ± 0.50 | kJ/mol | 370.50 | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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=C4076362&Units=SI |

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 |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| tt: | Triple Point Temperature |

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