# Thiourea, tetramethyl-

| | |
|---|---|
| **Other names:** | Urea, 1,1,3,3-tetramethyl-2-thio- |
| | Basthioryl |
| | N,N,N',N'-Tetramethylthiourea |
| | Tetramethylthiourea |
| | ((CH3)2N)2CS |
| | 1,1,3,3-Tetramethyl-2-thiourea |
| | 1,1,3,3-Tetramethylthiourea |
| | NA-101 |
| | TMTU |
| | Urea, thio-, tetramethyl- |
| | NSC 102499 |
| | Thiourea, N,N,N',N'-tetramethyl- |
| | tetramethyl-2-thiourea |
| **Inchi:** | InChI=1S/C5H12N2S/c1-6(2)5(8)7(3)4/h1-4H3 |
| **InchiKey:** | MNOILHPDHOHILI-UHFFFAOYSA-N |
| **Formula:** | C5H12N2S |
| **SMILES:** | CN(C)C(=S)N(C)C |
| **Mol. weight [g/mol]:** | 132.23 |
| **CAS:** | 2782-91-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 947.60 | kJ/mol | NIST Webbook |
| basg | 916.60 | kJ/mol | NIST Webbook |
| chs | -4246.70 ± 2.20 | kJ/mol | NIST Webbook |
| gf | 329.84 | kJ/mol | Joback Method |
| hf | 44.70 ± 2.30 | kJ/mol | NIST Webbook |
| hfs | -38.30 ± 2.30 | kJ/mol | NIST Webbook |
| hfus | 19.35 | kJ/mol | Joback Method |
| hsub | 83.00 ± 0.20 | kJ/mol | NIST Webbook |
| hsub | 85.00 ± 3.00 | kJ/mol | NIST Webbook |
| hsub | 84.00 | kJ/mol | NIST Webbook |
| hsub | 83.00 ± 0.50 | kJ/mol | NIST Webbook |
| hsub | 83.03 ± 0.20 | kJ/mol | NIST Webbook |
| hvap | 37.54 | kJ/mol | Joback Method |
| ie | 7.82 ± 0.03 | eV | NIST Webbook |
| ie | 7.84 | eV | NIST Webbook |

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|---|---|---|---|
| ie | 7.95 ± 0.05 | eV | NIST Webbook |
| ie | 7.84 | eV | NIST Webbook |
| ie | 7.82 | eV | NIST Webbook |
| log10ws | -0.40 | | Crippen Method |
| logp | 0.395 | | Crippen Method |
| mcvol | 113.320 | ml/mol | McGowan Method |
| pc | 3857.88 | kPa | Joback Method |
| ripol | 1872.00 | | NIST Webbook |
| tb | 408.72 | K | Joback Method |
| tc | 600.29 | K | Joback Method |
| tf | 245.32 | K | Joback Method |
| vc | 0.388 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 264.36 | J/mol×K | 568.36 | Joback Method |
| cpg | 211.55 | J/mol×K | 408.72 | Joback Method |
| cpg | 223.58 | J/mol×K | 440.65 | Joback Method |
| cpg | 234.83 | J/mol×K | 472.58 | Joback Method |
| cpg | 245.35 | J/mol×K | 504.51 | Joback Method |
| cpg | 255.18 | J/mol×K | 536.44 | Joback Method |
| cpg | 272.95 | J/mol×K | 600.29 | Joback Method |
| hfust | 22.14 | kJ/mol | 350.40 | NIST Webbook |
| hsubt | 83.00 ± 3.00 | kJ/mol | 333.00 | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2782914&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |