# Urea, N,N-dimethyl-N'-phenyl-

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|---|---|
| **Other names:** | 1,1-Dimethyl-3-phenylurea |
| | 1-Phenyl-3,3-dimethylurea |
| | 3-Phenyl-1,1-dimethylurea |
| | Amicure UR |
| | Dibar |
| | Dybar |
| | Dyhard RU 300 |
| | Dyhard UR 300 |
| | Falisilvan |
| | Fenidin |
| | Fenulon |
| | Fikure 62U |
| | N,N-Dimethyl-N'-phenylurea |
| | N-Phenyl-N',N'-dimethylurea |
| | Omicure 94 |
| | PDU |
| | PUD |
| | PUD (Herbicide) |
| | Urea, 1,1-dimethyl-3-phenyl- |
| | fenuron |
| **Inchi:** | InChI=1S/C9H12N2O/c1-11(2)9(12)10-8-6-4-3-5-7-8/h3-7H,1-2H3,(H,10,12) |
| **InchiKey:** | XXOYNJXVWVNOOJ-UHFFFAOYSA-N |
| **Formula:** | C9H12N2O |
| **SMILES:** | CN(C)C(=O)Nc1ccccc1 |
| **Mol. weight [g/mol]:** | 164.21 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -5054.30 ± 4.20 | kJ/mol | NIST Webbook |
| hf | -98.09 | kJ/mol | Cheméo Relay (1.0) |
| hfs | -203.00 ± 4.20 | kJ/mol | NIST Webbook |
| hfus | 22.83 | kJ/mol | Joback Method |
| hvap | 77.10 | kJ/mol | Cheméo Relay (1.0) |
| ie | 7.94 | eV | Cheméo Relay (1.0) |
| log10ws | -1.60 | | Aqueous Solubility Prediction Method |

| | | | |
|---|---|---|---|
| log10ws | -1.60 | | Estimated Solubility Method |
| logp | 1.780 | | Crippen Method |
| mcvol | 135.440 | ml/mol | McGowan Method |
| tb | 549.53 | K | Cheméo Relay (1.0) |
| tf | 406.53 | K | Aqueous Solubility Prediction Method |
| tf | 406.38 ± 0.20 | K | NIST Webbook |
| tf | 406.00 ± 0.20 | K | NIST Webbook |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 312.50 | J/mol×K | 548.48 | Joback Method |
| cpg | 326.22 | J/mol×K | 584.41 | Joback Method |
| cpg | 339.01 | J/mol×K | 620.35 | Joback Method |
| cpg | 350.93 | J/mol×K | 656.28 | Joback Method |
| cpg | 362.01 | J/mol×K | 692.21 | Joback Method |
| cpg | 372.29 | J/mol×K | 728.14 | Joback Method |
| cpg | 381.83 | J/mol×K | 764.08 | Joback Method |
| hfust | 22.81 | kJ/mol | 404.80 | NIST Webbook |
| hfust | 22.81 | kJ/mol | 404.80 | NIST Webbook |
| sfust | 59.77 | J/mol×K | 404.80 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C101428&Units=SI

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

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

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

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**Estimated Solubility Method:** http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **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 |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |