# IMIDODICARBONIC DIAMIDE

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|---|---|
| **Other names:** | Allophanamide |
| | Allophanic acid amide |
| | Allophanimidic acid |
| | Biuret |
| | Carbamylurea |
| | Dicarbamylamine |
| | Isobiuret |
| | Urea, (aminocarbonyl)- |
| | Ureidoformamide |
| | L-101 |
| | NSC 8020 |
| **Inchi:** | InChI=1S/C2H5N3O2/c3-1(6)5-2(4)7/h(H5,3,4,5,6,7) |
| **InchiKey:** | OHJMTUPIZMNBFR-UHFFFAOYSA-N |
| **Formula:** | C2H5N3O2 |
| **SMILES:** | NC(=O)NC(N)=O |
| **Mol. weight [g/mol]:** | 103.08 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -938.00 ± 2.10 | kJ/mol | NIST Webbook |
| hf | -437.00 ± 2.80 | kJ/mol | NIST Webbook |
| hfs | -563.70 ± 2.10 | kJ/mol | NIST Webbook |
| hfus | 19.63 | kJ/mol | Joback Method |
| hsub | 126.70 ± 1.90 | kJ/mol | NIST Webbook |
| hvap | 70.85 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.48 | eV | Cheméo Relay (1.0) |
| log10ws | -1.45 | | Cheméo Relay (1.0) |
| logp | -1.267 | | Crippen Method |
| mcvol | 72.120 | ml/mol | McGowan Method |
| ss | 146.10 | J/mol×K | NIST Webbook |
| ss | 146.10 | J/mol×K | NIST Webbook |
| tb | 491.22 | K | Cheméo Relay (1.0) |
| tf | 479.03 | K | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 162.19 | J/mol×K | 548.13 | Joback Method |
| cpg | 168.05 | J/mol×K | 585.63 | Joback Method |
| cpg | 173.53 | J/mol×K | 623.14 | Joback Method |
| cpg | 178.65 | J/mol×K | 660.64 | Joback Method |
| cpg | 183.39 | J/mol×K | 698.14 | Joback Method |
| cpg | 187.78 | J/mol×K | 735.64 | Joback Method |
| cpg | 191.83 | J/mol×K | 773.15 | Joback Method |
| cps | 131.30 | J/mol×K | 298.15 | NIST Webbook |
| cps | 131.30 | J/mol×K | 298.15 | NIST Webbook |

# Sources

**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
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C108190&Units=SI

# Legend

**chs:** Standard solid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**cps:** Solid phase 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
**hsub:** Enthalpy of sublimation at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient

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|---|---|
| **mcvol:** | McGowan's characteristic volume |
| **ss:** | Solid phase molar entropy at standard conditions |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |