

# Nitroguanidine

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Guanidine, nitro-<br>«alpha»-Nitroguanidine<br>«beta»-Nitroguanidine<br>N''-Nitroguanidine<br>Picrite<br>1-Nitroguanidine<br>Guanidine, 1-nitro-<br>Guanidine, 1-nitro- (wet)<br>Nitroguanidine, wet<br>N1-Nitroguanidine<br>Picrite (the explosive)<br>2-Nitroguanidine<br>Guanidine, N-nitro-<br>NSC 41036 |
| <b>Inchi:</b>               | InChI=1S/CH4N4O2/c2-1(3)4-5(6)7/h(H4,2,3,4)  |
| <b>InchiKey:</b>            | IDCPFAYURAQKDZ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | CH4N4O2  |
| <b>SMILES:</b>              | NC(N)=N[N+](=O)[O-]  |
| <b>Mol. weight [g/mol]:</b> | 104.07   |
| <b>CAS:</b>                 | 556-88-7   |

## Physical Properties

| Property code | Value          | Unit   | Source         |
|---------------|----------------|--------|----------------|
| chs           | -876.00        | kJ/mol | NIST Webbook   |
| chs           | -868.20 ± 4.20 | kJ/mol | NIST Webbook   |
| chs           | -866.90        | kJ/mol | NIST Webbook   |
| chs           | -878.60        | kJ/mol | NIST Webbook   |
| chs           | -896.20        | kJ/mol | NIST Webbook   |
| chs           | -872.80        | kJ/mol | NIST Webbook   |
| chs           | -879.00 ± 2.50 | kJ/mol | NIST Webbook   |
| hf            | 65.28          | kJ/mol | Joback Method  |
| hfs           | -97.90 ± 4.20  | kJ/mol | NIST Webbook   |
| hfs           | -89.10         | kJ/mol | NIST Webbook   |
| hfs           | -86.60 ± 2.50  | kJ/mol | NIST Webbook   |
| hsub          | 142.70 ± 2.00  | kJ/mol | NIST Webbook   |
| hvap          | 59.09          | kJ/mol | Joback Method  |
| log10ws       | -0.34          |        | Crippen Method |

|       |         |        |                |
|-------|---------|--------|----------------|
| logp  | -1.548  |        | Crippen Method |
| mcvol | 68.010  | ml/mol | McGowan Method |
| pc    | 6027.93 | kPa    | Joback Method  |
| tb    | 595.74  | K      | Joback Method  |
| tc    | 860.65  | K      | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source       |
|---------------|--------|---------|-----------------|--------------|
| cps           | 129.30 | J/mol×K | 298.00          | NIST Webbook |

## Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C556887&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C556887&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|                 |  |
|-----------------|--|
| <b>chs:</b>     | Standard solid enthalpy of combustion                    |
| <b>cps:</b>     | Solid phase heat capacity                                |
| <b>hf:</b>      | Enthalpy of formation at standard conditions             |
| <b>hfs:</b>     | Solid phase enthalpy of formation at standard conditions |
| <b>hsub:</b>    | Enthalpy of sublimation at standard conditions           |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions          |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l                       |
| <b>logp:</b>    | Octanol/Water partition coefficient                      |
| <b>mcvol:</b>   | McGowan's characteristic volume                          |
| <b>pc:</b>      | Critical Pressure  |
| <b>tb:</b>      | Normal Boiling Point Temperature                         |
| <b>tc:</b>      | Critical Temperature                                     |

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