

# Nitrogen oxide cation

|                      |                             |
|----------------------|-----------------------------|
| Inchi:               | InChI=1S/NO2/c2-1-3/q+1     |
| InchiKey:            | OMBRFUXPXNIUCZ-UHFFFAOYSA-N |
| Formula:             | N2O+                        |
| SMILES:              | O=[N+]=O                    |
| Mol. weight [g/mol]: | 44.01                       |
| CAS:                 | 12269-46-4                  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 37.05   | kJ/mol  | Joback Method  |
| hf            | 1.72    | kJ/mol  | Joback Method  |
| hfus          | 8.80    | kJ/mol  | Joback Method  |
| hvap          | 32.04   | kJ/mol  | Joback Method  |
| log10ws       | 3.81    |         | Crippen Method |
| logp          | -0.414  |         | Crippen Method |
| mcvol         | 26.130  | ml/mol  | McGowan Method |
| pc            | 7406.07 | kPa     | Joback Method  |
| tb            | 350.54  | K       | Joback Method  |
| tc            | 561.53  | K       | Joback Method  |
| tf            | 249.74  | K       | Joback Method  |
| vc            | 0.108   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value | Unit    | Temperature [K] | Source        |
|---------------|-------|---------|-----------------|---------------|
| cpg           | 33.13 | J/mol×K | 350.54          | Joback Method |
| cpg           | 35.27 | J/mol×K | 385.70          | Joback Method |
| cpg           | 37.11 | J/mol×K | 420.87          | Joback Method |
| cpg           | 38.66 | J/mol×K | 456.03          | Joback Method |
| cpg           | 39.96 | J/mol×K | 491.20          | Joback Method |
| cpg           | 41.04 | J/mol×K | 526.36          | Joback Method |
| cpg           | 41.93 | J/mol×K | 561.53          | Joback Method |

# Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <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=C12269464&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C12269464&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion 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                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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