# 2-Methyl-6-nitroaniline

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|---|---|
| **Other names:** | 2-Amino-3-nitrotoluene |
| | 6-Nitro-o-toluidine |
| | Benzenamine, 2-methyl-6-nitro- |
| | aniline, 2-methyl-6-nitro- |
| **Inchi:** | InChI=1S/C7H8N2O2/c1-5-3-2-4-6(7(5)8)9(10)11/h2-4H,8H2,1H3 |
| **InchiKey:** | FCMRHMPITHLLLA-UHFFFAOYSA-N |
| **Formula:** | C7H8N2O2 |
| **SMILES:** | Cc1cccc([N+](=O)[O-])c1N |
| **Mol. weight [g/mol]:** | 152.15 |
| **CAS:** | 570-24-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 203.21 | kJ/mol | Joback Method |
| hf | 48.81 | kJ/mol | Joback Method |
| hfus | 23.71 | kJ/mol | Joback Method |
| hvap | 62.01 | kJ/mol | Joback Method |
| log10ws | -2.23 | | Crippen Method |
| logp | 1.485 | | Crippen Method |
| mcvol | 113.130 | ml/mol | McGowan Method |
| pc | 4328.25 | kPa | Joback Method |
| tb | 620.57 | K | Joback Method |
| tc | 879.01 | K | Joback Method |
| tf | 366.75 | K | Solubility and solution thermodynamics of 2-methyl-6-nitroaniline in ten organic solvents at elevated temperatures |
| vc | 0.430 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 269.53 | J/mol×K | 620.57 | Joback Method |
| cpg | 280.15 | J/mol×K | 663.64 | Joback Method |

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|---|---|---|---|---|
| cpg | 289.96 | J/mol×K | 706.72 | Joback Method |
| cpg | 299.00 | J/mol×K | 749.79 | Joback Method |
| cpg | 307.29 | J/mol×K | 792.87 | Joback Method |
| cpg | 314.89 | J/mol×K | 835.94 | Joback Method |
| cpg | 321.82 | J/mol×K | 879.01 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.25107e+01 |
| Coeff. B | -3.79209e+03 |
| Coeff. C | -8.72810e+01 |
| Temperature range (K), min. | 397.52 |
| Temperature range (K), max. | 614.02 |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Solubility and solution thermodynamics of 2-methyl-6-nitroaniline in ten organic solvents at elevated temperatures:** | https://www.doi.org/10.1016/j.jct.2016.05.027 |
| **Determination and thermodynamic modeling for 2-methyl-6-nitroaniline solubility in binary solvent mixtures of ethyl acetate + (methanol, ethanol, n-propanol and isopropanol):** | https://www.doi.org/10.1016/j.jct.2016.10.043 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C570241&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |