# 2,4,6-Trinitro-N-methyl-aniline

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|---|---|
| **Other names:** | Benzenamine, N-methyl-2,4,6-trinitro-<br>Aniline, N-methyl-2,4,6-trinitro-<br>N-Methyl-2,4,6-trinitroaniline<br>N-Methylpicramide |
| **Inchi:** | InChI=1S/C7H6N4O6/c1-8-7-5(10(14)15)2-4(9(12)13)3-6(7)11(16)17/h2-3,8H,1H3 |
| **InchiKey:** | CFYAUGJHWXGWHI-UHFFFAOYSA-N |
| **Formula:** | C7H6N4O6 |
| **SMILES:** | CNc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-] |
| **Mol. weight [g/mol]:** | 242.15 |
| **CAS:** | 1022-07-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3562.80 ± 2.40 | kJ/mol | NIST Webbook |
| gf | 287.62 | kJ/mol | Joback Method |
| hf | 35.50 | kJ/mol | Joback Method |
| hfs | -49.30 ± 3.60 | kJ/mol | NIST Webbook |
| hfus | 45.94 | kJ/mol | Joback Method |
| hvap | 91.65 | kJ/mol | Joback Method |
| log10ws | -3.43 | | Crippen Method |
| logp | 1.453 | | Crippen Method |
| mcvol | 147.970 | ml/mol | McGowan Method |
| pc | 4135.61 | kPa | Joback Method |
| tb | 906.87 | K | Joback Method |
| tc | 1190.19 | K | Joback Method |
| tf | 716.12 | K | Joback Method |
| vc | 0.601 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 415.26 | J/mol×K | 906.87 | Joback Method |
| cpg | 422.37 | J/mol×K | 954.09 | Joback Method |
| cpg | 428.56 | J/mol×K | 1001.31 | Joback Method |

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|---|---|---|---|---|
| cpg | 433.89 | J/mol×K | 1048.53 | Joback Method |
| cpg | 438.43 | J/mol×K | 1095.75 | Joback Method |
| cpg | 442.23 | J/mol×K | 1142.97 | Joback Method |
| cpg | 445.34 | J/mol×K | 1190.19 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1022077&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |