# Benzenamine, N,N,2-trimethyl-

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|---|---|
| **Other names:** | 2,N,N-Trimethylaniline |
| | 2-Methyl-N,N-dimethylaniline |
| | Benzene, 1-(dimethylamino)-2-methyl- |
| | Benzeneamine,N,N,2-trimethyl- |
| | Dimethyl-o-toluidine |
| | N,N'-dimethyl-o-toluidine |
| | N,N,2-TRIMETHYLANILINE |
| | N,N,2-Trimethylbenzenamine |
| | N,N-DIMETHYL-O-TOLUIDINE |
| | N,N-Dimethyl-2-methylaniline |
| | NSC 1784 |
| | O-METHYLDIMETHYLANILINE |
| | o-Toluidine, N,N-dimethyl- |
| **Inchi:** | InChI=1S/C9H13N/c1-8-6-4-5-7-9(8)10(2)3/h4-7H,1-3H3 |
| **InchiKey:** | JDEJGVSZUIJWBM-UHFFFAOYSA-N |
| **Formula:** | C9H13N |
| **SMILES:** | Cc1ccccc1N(C)C |
| **Mol. weight [g/mol]:** | 135.21 |
| **CAS:** | 609-72-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 951.80 | kJ/mol | NIST Webbook |
| basg | 925.30 | kJ/mol | NIST Webbook |
| gf | 238.46 | kJ/mol | Joback Method |
| hf | 63.50 | kJ/mol | Joback Method |
| hfus | 15.74 | kJ/mol | Joback Method |
| hvap | 40.61 | kJ/mol | Joback Method |
| ie | 7.37 | eV | NIST Webbook |
| ie | 7.92 | eV | NIST Webbook |
| ie | 7.44 | eV | NIST Webbook |
| ie | 7.92 | eV | NIST Webbook |
| ie | 7.40 ± 0.02 | eV | NIST Webbook |
| ie | 7.42 ± 0.02 | eV | NIST Webbook |
| log10ws | -1.86 | | Crippen Method |
| logp | 2.061 | | Crippen Method |
| mcvol | 123.890 | ml/mol | McGowan Method |

| | | | |
|---|---|---|---|
| pc | 3120.81 ± 101.32 | kPa | NIST Webbook |
| pc | 3120.81 ± 101.32 | kPa | NIST Webbook |
| pc | 3120.00 ± 91.19 | kPa | NIST Webbook |
| rinpol | 1164.60 | | NIST Webbook |
| tb | 458.65 ± 0.50 | K | NIST Webbook |
| tb | 458.45 ± 0.30 | K | NIST Webbook |
| tb | 458.45 ± 0.35 | K | NIST Webbook |
| tb | 458.50 | K | NIST Webbook |
| tc | 667.80 ± 2.50 | K | NIST Webbook |
| tc | 667.95 ± 1.00 | K | NIST Webbook |
| tc | 667.95 ± 1.00 | K | NIST Webbook |
| tf | 211.85 ± 0.70 | K | NIST Webbook |
| tf | 213.15 ± 0.70 | K | NIST Webbook |
| vc | 0.450 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 246.45 | J/mol×K | 449.42 | Joback Method |
| cpg | 261.05 | J/mol×K | 483.73 | Joback Method |
| cpg | 274.83 | J/mol×K | 518.04 | Joback Method |
| cpg | 287.83 | J/mol×K | 552.35 | Joback Method |
| cpg | 300.07 | J/mol×K | 586.67 | Joback Method |
| cpg | 311.58 | J/mol×K | 620.98 | Joback Method |
| cpg | 322.41 | J/mol×K | 655.29 | Joback Method |
| hvapt | 52.40 | kJ/mol | 379.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.45470e+01 |
| Coeff. B | -3.83224e+03 |
| Coeff. C | -7.25250e+01 |
| Temperature range (K), min. | 341.28 |
| Temperature range (K), max. | 487.47 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 1.36661e+02 |
| Coeff. B | -1.11966e+04 |
| Coeff. C | -1.79824e+01 |
| Coeff. D | 1.22854e-05 |
| Temperature range (K), min. | 301.15 |
| Temperature range (K), max. | 458.15 |

# Sources

| | |
|---|---|
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1308.mol |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C609723&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1308 |
| **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

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |

| | |
|---|---|
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |