# 1,2-Ethanediamine, N,N,N'-trimethyl-

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| **Other names:** | 1,2-Diaminoethane, N,N,N'-trimethyl-<br>1-(N,N-dimethylamino)-2-(N-methylamino)ethane<br>2-(Dimethylamino)-N-methylethylamine<br>Ethylenediamine, N,N,N'-trimethyl-<br>N,N,N'-Trimethyl-1,2-ethanediamine<br>N,N,N'-Trimethyldiaminoethane<br>N,N,N'-Trimethylethanediamine<br>N,N,N'-Trimethylethylenediamine<br>N-[2-(dimethylamino)ethyl]-N-methylamine<br>N1,N1,N2-trimethylethane-1,2-diamine<br>dimethyl(2-(methylamino)ethyl)amine |
| **Inchi:** | InChI=1S/C5H14N2/c1-6-4-5-7(2)3/h6H,4-5H2,1-3H3 |
| **InchiKey:** | HVOYZOQVDYHUPF-UHFFFAOYSA-N |
| **Formula:** | C5H14N2 |
| **SMILES:** | CNCCN(C)C |
| **Mol. weight [g/mol]:** | 102.18 |
| **CAS:** | 142-25-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 191.39 | kJ/mol | Joback Method |
| hf | -25.53 | kJ/mol | Joback Method |
| hfus | 16.83 | kJ/mol | Joback Method |
| hvap | 35.20 | kJ/mol | Joback Method |
| log10ws | 0.33 | | Crippen Method |
| logp | -0.233 | | Crippen Method |
| mcvol | 101.270 | ml/mol | McGowan Method |
| pc | 3513.74 | kPa | Joback Method |
| tb | 390.20 | K | NIST Webbook |
| tc | 545.47 | K | Joback Method |
| tf | 231.24 | K | Joback Method |
| vc | 0.368 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 250.59 | J/mol×K | 545.47 | Joback Method |
| cpg | 231.85 | J/mol×K | 489.11 | Joback Method |
| cpg | 221.84 | J/mol×K | 460.94 | Joback Method |
| cpg | 211.39 | J/mol×K | 432.76 | Joback Method |
| cpg | 200.50 | J/mol×K | 404.59 | Joback Method |
| cpg | 189.13 | J/mol×K | 376.41 | Joback Method |
| cpg | 241.43 | J/mol×K | 517.29 | Joback Method |
| cpl | 265.30 | J/mol×K | 318.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| cpl | 269.20 | J/mol×K | 323.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| cpl | 260.00 | J/mol×K | 308.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| cpl | 258.30 | J/mol×K | 303.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |

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| cpl | 272.70 | J/mol×K | 328.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| cpl | 276.00 | J/mol×K | 333.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| cpl | 278.90 | J/mol×K | 338.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| cpl | 281.30 | J/mol×K | 343.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| cpl | 283.40 | J/mol×K | 348.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |

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| cpl | 262.70 | J/mol×K | 313.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| cpl | 286.60 | J/mol×K | 353.20 | Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)-piperazine and N,N,N'-trimethylethylenediamine at temperatures (303.2-353.2) K |
| pvap | 4.40 | kPa | 305.40 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 4.07 | kPa | 304.10 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 3.81 | kPa | 303.20 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 3.26 | kPa | 301.00 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 2.73 | kPa | 298.20 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |

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| pvap | 2.40 | kPa | 296.30 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 1.69 | kPa | 291.00 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 1.27 | kPa | 286.80 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 0.89 | kPa | 281.80 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 0.60 | kPa | 276.70 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |
| pvap | 0.50 | kPa | 274.20 | Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.56393e+01 |
| Coeff. B | -3.75363e+03 |
| Coeff. C | -4.96120e+01 |
| Temperature range (K), min. | 294.12 |
| Temperature range (K), max. | 413.06 |

# Sources

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|---|---|
| **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 |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl) piperazine and N,N,N′-trimethylethylenediamine at temperatures (303.2–353.2) K:** | https://www.doi.org/10.1016/j.jct.2016.08.006 |
| **Thermodynamic Properties of N-Methyl-Substituted Ethylenediamines: Experimental and Computational Study:** | https://www.doi.org/10.1021/acs.jced.5b01003 |
| **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=C142256&Units=SI |

# Legend

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| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase 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 |
| **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 |