# N-Ethyl trimethylenediamine

**Inchi:** InChI=1S/C5H14N2/c1-2-7-5-3-4-6/h7H,2-6H2,1H3
**InchiKey:** ODGYWRBCQWKSSH-UHFFFAOYSA-N
**Formula:** C5H14N2
**SMILES:** CCNCCCN
**Mol. weight [g/mol]:** 102.18
**CAS:** 38571-87-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 147.06 | kJ/mol | Joback Method |
| hf | -59.27 | kJ/mol | Joback Method |
| hfus | 19.00 | kJ/mol | Joback Method |
| hvap | 43.80 | kJ/mol | Joback Method |
| log10ws | -0.54 | | Crippen Method |
| logp | -0.055 | | Crippen Method |
| mcvol | 101.270 | ml/mol | McGowan Method |
| pc | 3773.04 | kPa | Joback Method |
| tb | 436.50 | K | Joback Method |
| tc | 621.90 | K | Joback Method |
| tf | 282.03 | K | Joback Method |
| vc | 0.380 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 213.90 | J/mol×K | 436.50 | Joback Method |
| cpg | 224.78 | J/mol×K | 467.40 | Joback Method |
| cpg | 235.20 | J/mol×K | 498.30 | Joback Method |
| cpg | 245.17 | J/mol×K | 529.20 | Joback Method |
| cpg | 254.70 | J/mol×K | 560.10 | Joback Method |
| cpg | 263.81 | J/mol×K | 591.00 | Joback Method |
| cpg | 272.50 | J/mol×K | 621.90 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C38571878&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **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 |