# Bis(2-chloroethyl)ethylamine

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|---|---|
| **Other names:** | 2,2'-Dichlorotriethylamine |
| | Ethanamine, 2-chloro-N-(2-chloroethyl)-N-ethyl- |
| | Ethyl-S |
| | Ethylbis(2-chloroethyl)amine |
| | Ethylbis(«beta»-chloroethyl)amine |
| | Ethylbis(Â«betaÂ»-chloroethyl)amine |
| | HN1 |
| | Nitrogen mustard (HN-1) |
| | TL 1149 |
| | TL 329 |
| | Triethylamine, 2,2'-dichloro- |
| **Inchi:** | InChI=1S/C6H13Cl2N/c1-2-9(5-3-7)6-4-8/h2-6H2,1H3 |
| **InchiKey:** | UQZPGHOJMQTOHB-UHFFFAOYSA-N |
| **Formula:** | C6H13Cl2N |
| **SMILES:** | CCN(CCCl)CCCl |
| **Mol. weight [g/mol]:** | 170.08 |
| **CAS:** | 538-07-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 86.56 | kJ/mol | Joback Method |
| hf | -131.12 | kJ/mol | Joback Method |
| hfus | 22.71 | kJ/mol | Joback Method |
| hvap | 39.76 | kJ/mol | Joback Method |
| log10ws | -1.21 | | Crippen Method |
| logp | 1.786 | | Crippen Method |
| mcvol | 129.860 | ml/mol | McGowan Method |
| pc | 2859.68 | kPa | Joback Method |
| rinpol | 1156.00 | | NIST Webbook |
| tb | 423.98 | K | Joback Method |
| tc | 602.32 | K | Joback Method |
| tf | 249.69 | K | Joback Method |
| vc | 0.487 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 240.95 | J/mol×K | 423.98 | Joback Method |
| cpg | 252.18 | J/mol×K | 453.70 | Joback Method |
| cpg | 262.89 | J/mol×K | 483.43 | Joback Method |
| cpg | 273.08 | J/mol×K | 513.15 | Joback Method |
| cpg | 282.79 | J/mol×K | 542.87 | Joback Method |
| cpg | 292.02 | J/mol×K | 572.60 | Joback Method |
| cpg | 300.80 | J/mol×K | 602.32 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.25244e+01 |
| Coeff. B | -4.37791e+03 |
| Temperature range (K), min. | 357.77 |
| Temperature range (K), max. | 606.96 |

# Sources

**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=C538078&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

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

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