# 2-Pentanamine, 4-methyl-

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|---|---|
| **Other names:** | 1,3-Dimethyl-n-butylamine |
| | 1,3-Dimethylbutanamine |
| | 1,3-Dimethylbutylamine |
| | 2-Amino-4-methylpentane |
| | 4-Methyl-2-aminopentane |
| | Butylamine, 1,3-dimethyl- |
| | UN 2379 |
| **Inchi:** | InChI=1S/C6H15N/c1-5(2)4-6(3)7/h5-6H,4,7H2,1-3H3 |
| **InchiKey:** | UNBMPKNTYKDYCG-UHFFFAOYSA-N |
| **Formula:** | C6H15N |
| **SMILES:** | CC(C)CC(C)N |
| **Mol. weight [g/mol]:** | 101.19 |
| **CAS:** | 108-09-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 61.21 | kJ/mol | Joback Method |
| hf | -143.94 | kJ/mol | Joback Method |
| hfus | 9.45 | kJ/mol | Joback Method |
| hvap | 38.81 | kJ/mol | Joback Method |
| log10ws | -1.64 | | Crippen Method |
| logp | 1.380 | | Crippen Method |
| mcvol | 105.380 | ml/mol | McGowan Method |
| pc | 3376.28 | kPa | Joback Method |
| tb | 351.15 ± 2.00 | K | NIST Webbook |
| tb | 382.20 | K | NIST Webbook |
| tc | 596.83 | K | Joback Method |
| tf | 210.64 | K | Joback Method |
| vc | 0.389 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 211.00 | J/mol×K | 408.33 | Joback Method |

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|---|---|---|---|---|
| cpg | 223.15 | J/mol×K | 439.75 | Joback Method |
| cpg | 234.78 | J/mol×K | 471.16 | Joback Method |
| cpg | 245.91 | J/mol×K | 502.58 | Joback Method |
| cpg | 256.56 | J/mol×K | 534.00 | Joback Method |
| cpg | 266.73 | J/mol×K | 565.41 | Joback Method |
| cpg | 276.44 | J/mol×K | 596.83 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.39086e+01 |
| Coeff. B | -2.73098e+03 |
| Coeff. C | -8.82400e+01 |
| Temperature range (K), min. | 288.74 |
| Temperature range (K), max. | 405.90 |

# Sources

**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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C108098&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |