# 1-Propanamine, 2-methyl-N-(2-methylpropyl)-

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|---|---|
| **Other names:** | (i-C4H9)2NH |
| | DI(-2-METHYLPROPYL)AMINE |
| | Diisobutylamine |
| | N,N-Bis(2-methylpropyl)amine |
| | UN 2361 |
| **Inchi:** | InChI=1S/C8H19N/c1-7(2)5-9-6-8(3)4/h7-9H,5-6H2,1-4H3 |
| **InchiKey:** | NJBCRXCAPCODGX-UHFFFAOYSA-N |
| **Formula:** | C8H19N |
| **SMILES:** | CC(C)CNCC(C)C |
| **Mol. weight [g/mol]:** | 129.24 |
| **CAS:** | 110-96-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5480 | | KDB |
| affp | 958.10 | kJ/mol | NIST Webbook |
| basg | 925.10 | kJ/mol | NIST Webbook |
| chl | -5644.93 ± 0.42 | kJ/mol | NIST Webbook |
| chl | -5638.10 ± 2.00 | kJ/mol | NIST Webbook |
| chl | -5663.50 | kJ/mol | NIST Webbook |
| gf | 100.99 | kJ/mol | Joback Method |
| hf | -180.80 ± 2.70 | kJ/mol | NIST Webbook |
| hf | -174.00 | kJ/mol | NIST Webbook |
| hf | -191.40 | kJ/mol | NIST Webbook |
| hfl | -225.40 ± 2.30 | kJ/mol | NIST Webbook |
| hfl | -218.60 ± 0.46 | kJ/mol | NIST Webbook |
| hfl | -236.00 | kJ/mol | NIST Webbook |
| hfus | 14.53 | kJ/mol | Joback Method |
| hvap | 43.10 ± 0.30 | kJ/mol | NIST Webbook |
| hvap | 44.60 | kJ/mol | NIST Webbook |
| hvap | 39.30 | kJ/mol | NIST Webbook |
| hvap | 44.60 ± 1.50 | kJ/mol | NIST Webbook |
| ie | 7.80 | eV | NIST Webbook |
| log10ws | -1.88 | | Crippen Method |
| logp | 1.888 | | Crippen Method |
| mcvol | 133.560 | ml/mol | McGowan Method |
| pc | 3200.00 | kPa | KDB |

| | | | |
|---|---|---|---|
| pc | 3200.00 ± 31.97 | kPa | NIST Webbook |
| rinpol | 850.00 | | NIST Webbook |
| rinpol | 850.00 | | NIST Webbook |
| rinpol | 849.00 | | NIST Webbook |
| tb | 412.70 | K | NIST Webbook |
| tb | 411.95 ± 0.60 | K | NIST Webbook |
| tb | 411.65 ± 0.60 | K | NIST Webbook |
| tb | 412.50 ± 0.50 | K | NIST Webbook |
| tb | 412.84 | K | KDB |
| tb | 411.20 | K | NIST Webbook |
| tb | 412.65 ± 2.00 | K | NIST Webbook |
| tc | 584.40 | K | KDB |
| tc | 584.40 ± 0.58 | K | NIST Webbook |
| tf | 199.60 | K | KDB |
| tf | 196.00 | K | NIST Webbook |
| tf | 199.65 ± 0.50 | K | NIST Webbook |
| tf | 203.15 ± 0.50 | K | NIST Webbook |
| vc | 0.506 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 320.91 | J/mol×K | 519.67 | Joback Method |
| cpg | 333.62 | J/mol×K | 548.99 | Joback Method |
| cpg | 345.79 | J/mol×K | 578.30 | Joback Method |
| cpg | 279.42 | J/mol×K | 431.73 | Joback Method |
| cpg | 293.82 | J/mol×K | 461.04 | Joback Method |
| cpg | 307.65 | J/mol×K | 490.36 | Joback Method |
| cpg | 357.44 | J/mol×K | 607.62 | Joback Method |
| hvapt | 43.80 | kJ/mol | 340.50 | NIST Webbook |
| hvapt | 39.00 | kJ/mol | 291.00 | NIST Webbook |
| rhol | 741.00 | kg/m3 | 298.00 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |

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|---|---|
| Coeff. A | 1.56848e+01 |
| Coeff. B | -3.94237e+03 |
| Coeff. C | -5.57550e+01 |
| Temperature range (K), min. | 311.80 |
| Temperature range (K), max. | 435.80 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 4.69121e+01 |
| Coeff. B | -6.47642e+03 |
| Coeff. C | -4.44104e+00 |
| Coeff. D | 1.29328e-06 |
| Temperature range (K), min. | 203.15 |
| Temperature range (K), max. | 584.00 |

# Sources

| | |
|---|---|
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1275.mol |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C110963&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=1275 |
| **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

| | |
|---|---|
| **af:** | Acentric Factor |
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase 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 |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |