# 1-Butanamine, N-(1-methylethyl)-

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|---|---|
| **Other names:** | Butylisopropylamine<br>Isopropylbutylamine<br>N-Isopropylbutylamine<br>Butylamine, N-isopropyl-<br>isopropyl-n-butylamine |
| **Inchi:** | InChI=1S/C7H17N/c1-4-5-6-8-7(2)3/h7-8H,4-6H2,1-3H3 |
| **InchiKey:** | OKRJGUKZYSEUOY-UHFFFAOYSA-N |
| **Formula:** | C7H17N |
| **SMILES:** | CCCCNC(C)C |
| **Mol. weight [g/mol]:** | 115.22 |
| **CAS:** | 39099-23-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -4980.90 ± 3.00 | kJ/mol | NIST Webbook |
| gf | 95.01 | kJ/mol | Joback Method |
| hf | -165.00 ± 3.70 | kJ/mol | NIST Webbook |
| hfl | -203.20 ± 3.10 | kJ/mol | NIST Webbook |
| hfus | 15.46 | kJ/mol | Joback Method |
| hvap | 42.10 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 38.20 | kJ/mol | NIST Webbook |
| hvap | 42.08 | kJ/mol | NIST Webbook |
| hvap | 38.20 ± 2.00 | kJ/mol | NIST Webbook |
| log10ws | -2.05 | | Crippen Method |
| logp | 1.785 | | Crippen Method |
| mcvol | 119.470 | ml/mol | McGowan Method |
| pc | 2862.74 | kPa | Joback Method |
| rinpol | 795.00 | | NIST Webbook |
| rinpol | 795.00 | | NIST Webbook |
| tb | 396.60 | K | NIST Webbook |
| tb | 397.15 ± 2.00 | K | NIST Webbook |
| tc | 563.60 | K | NIST Webbook |
| tf | 206.31 | K | Joback Method |
| vc | 0.457 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 308.53 | J/mol×K | 582.34 | Joback Method |
| cpg | 251.08 | J/mol×K | 438.13 | Joback Method |
| cpg | 263.53 | J/mol×K | 466.97 | Joback Method |
| cpg | 275.48 | J/mol×K | 495.82 | Joback Method |
| cpg | 286.96 | J/mol×K | 524.66 | Joback Method |
| cpg | 297.97 | J/mol×K | 553.50 | Joback Method |
| cpg | 238.14 | J/mol×K | 409.29 | Joback Method |
| hvapt | 34.52 | kJ/mol | 396.60 | NIST Webbook |
| hvapt | 40.90 ± 0.10 | kJ/mol | 313.00 | NIST Webbook |
| hvapt | 39.90 ± 0.10 | kJ/mol | 328.00 | NIST Webbook |
| hvapt | 38.70 ± 0.10 | kJ/mol | 343.00 | NIST Webbook |
| hvapt | 37.60 ± 0.10 | kJ/mol | 358.00 | NIST Webbook |
| hvapt | 40.00 | kJ/mol | 360.00 | NIST Webbook |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C39099235&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

| | |
|---|---|
| **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 |
| **log10ws:** | Log10 of Water solubility in mol/l |

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|---|---|
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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