# 3-Butyn-2-amine, 2-methyl-

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|---|---|
| **Other names:** | 3-Amino-3-methyl-1-butyne |
| | 1,1-Dimethylpropargylamine |
| | 1,1-dimethylprop-3-ynylamine |
| **Inchi:** | InChI=1S/C5H9N/c1-4-5(2,3)6/h1H,6H2,2-3H3 |
| **InchiKey:** | VUGCBIWQHSRQBZ-UHFFFAOYSA-N |
| **Formula:** | C5H9N |
| **SMILES:** | C#CC(C)(C)N |
| **Mol. weight [g/mol]:** | 83.13 |
| **CAS:** | 2978-58-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 283.58 | kJ/mol | Joback Method |
| hf | 170.41 | kJ/mol | Joback Method |
| hfus | 9.46 | kJ/mol | Joback Method |
| hvap | 35.93 | kJ/mol | Joback Method |
| log10ws | -1.26 | | Crippen Method |
| logp | 0.357 | | Crippen Method |
| mcvol | 82.690 | ml/mol | McGowan Method |
| pc | 4602.62 | kPa | Joback Method |
| tb | 352.70 | K | NIST Webbook |
| tc | 581.72 | K | Joback Method |
| tf | 278.76 | K | Joback Method |
| vc | 0.295 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 151.66 | J/mol×K | 373.22 | Joback Method |
| cpg | 161.47 | J/mol×K | 407.97 | Joback Method |
| cpg | 170.61 | J/mol×K | 442.72 | Joback Method |
| cpg | 179.12 | J/mol×K | 477.47 | Joback Method |
| cpg | 187.05 | J/mol×K | 512.22 | Joback Method |
| cpg | 194.42 | J/mol×K | 546.97 | Joback Method |

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|---|---|---|---|---|
| cpg | 201.27 | J/mol×K | 581.72 | Joback Method |

# Sources

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|---|---|
| **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=C2978587&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |