# 1-Pentyne

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|---|---|
| **Other names:** | Acetylene, propyl- |
| | C3H7C«equiv»CH |
| | C3H7CÂ«equivÂ»CH |
| | PROPYLACETYLENE |
| | pent-1-yne |
| **Inchi:** | InChI=1S/C5H8/c1-3-5-4-2/h1H,4-5H2,2H3 |
| **InchiKey:** | IBXNCJKFFQIKKY-UHFFFAOYSA-N |
| **Formula:** | C5H8 |
| **SMILES:** | C#CCCC |
| **Mol. weight [g/mol]:** | 68.12 |
| **CAS:** | 627-19-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.1640 | | KDB |
| dm | 0.90 | debye | KDB |
| gf | 210.40 | kJ/mol | KDB |
| hcg | 3226.62 | kJ/mol | KDB |
| hcn | 3050.554 | kJ/mol | KDB |
| hf | 144.30 ± 2.10 | kJ/mol | NIST Webbook |
| hf | 144.40 | kJ/mol | KDB |
| hfus | 11.68 | kJ/mol | Joback Method |
| hvap | 28.40 | kJ/mol | NIST Webbook |
| ie | 10.10 ± 0.01 | eV | NIST Webbook |
| ie | 10.10 ± 0.02 | eV | NIST Webbook |
| ie | 10.10 ± 0.01 | eV | NIST Webbook |
| ie | 10.05 | eV | NIST Webbook |
| log10ws | -1.64 | | Estimated Solubility Method |
| log10ws | -1.64 | | Aqueous Solubility Prediction Method |
| logp | 1.420 | | Crippen Method |
| mcvol | 72.710 | ml/mol | McGowan Method |
| pc | 4050.00 | kPa | KDB |
| rinpol | 509.00 | | NIST Webbook |
| rinpol | 484.00 | | NIST Webbook |
| rinpol | 484.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 484.50 | | NIST Webbook |
| rinpol | 484.00 | | NIST Webbook |
| rinpol | 510.00 | | NIST Webbook |
| rinpol | 484.40 | | NIST Webbook |
| rinpol | 509.00 | | NIST Webbook |
| rinpol | 484.00 | | NIST Webbook |
| rinpol | 484.50 | | NIST Webbook |
| rinpol | 484.00 | | NIST Webbook |
| rinpol | 484.00 | | NIST Webbook |
| rinpol | 484.80 | | NIST Webbook |
| rinpol | 517.00 | | NIST Webbook |
| rinpol | 484.00 | | NIST Webbook |
| rinpol | 484.00 | | NIST Webbook |
| rinpol | 484.40 | | NIST Webbook |
| tb | 312.95 ± 1.00 | K | NIST Webbook |
| tb | 313.15 ± 1.00 | K | NIST Webbook |
| tb | 313.15 ± 1.50 | K | NIST Webbook |
| tb | 312.90 ± 0.80 | K | NIST Webbook |
| tb | 313.15 ± 0.70 | K | NIST Webbook |
| tb | 312.15 ± 1.00 | K | NIST Webbook |
| tb | 312.85 ± 0.60 | K | NIST Webbook |
| tb | 313.15 ± 1.00 | K | NIST Webbook |
| tb | 312.45 ± 0.50 | K | NIST Webbook |
| tb | 312.65 ± 1.50 | K | NIST Webbook |
| tb | 313.35 ± 0.30 | K | NIST Webbook |
| tb | 315.15 ± 2.00 | K | NIST Webbook |
| tb | 313.40 ± 0.20 | K | NIST Webbook |
| tb | 313.35 ± 0.40 | K | NIST Webbook |
| tb | 312.65 ± 2.00 | K | NIST Webbook |
| tb | 313.33 ± 0.20 | K | NIST Webbook |
| tb | 313.38 ± 0.20 | K | NIST Webbook |
| tb | 312.80 ± 2.00 | K | NIST Webbook |
| tb | 313.40 | K | NIST Webbook |
| tb | 313.00 | K | NIST Webbook |
| tb | 313.33 | K | KDB |
| tb | 312.20 ± 1.00 | K | NIST Webbook |
| tb | 312.85 ± 1.00 | K | NIST Webbook |
| tc | 493.50 | K | KDB |
| tf | 183.00 | K | KDB |
| tf | 167.08 ± 0.20 | K | NIST Webbook |
| tf | 166.65 ± 0.30 | K | NIST Webbook |
| tf | 172.48 | K | Aqueous Solubility Prediction Method |
| vc | 0.278 | m3/kmol | KDB |
| zc | 0.2743950 | | KDB |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 115.69 | J/mol×K | 332.98 | Joback Method |
| cpg | 122.65 | J/mol×K | 362.05 | Joback Method |
| cpg | 129.31 | J/mol×K | 391.11 | Joback Method |
| cpg | 135.70 | J/mol×K | 420.17 | Joback Method |
| cpg | 141.82 | J/mol×K | 449.24 | Joback Method |
| cpg | 108.43 | J/mol×K | 303.92 | Joback Method |
| cpg | 147.68 | J/mol×K | 478.30 | Joback Method |
| hvapt | 27.74 | kJ/mol | 313.40 | KDB |
| hvapt | 31.80 | kJ/mol | 272.00 | NIST Webbook |
| rfi | 1.38260 | | 298.15 | KDB |
| rhol | 690.00 | kg/m3 | 293.00 | KDB |
| srf | 0.02 | N/m | 298.20 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.39994e+01 |
| Coeff. B | -2.38534e+03 |
| Coeff. C | -5.90590e+01 |
| Temperature range (K), min. | 233.02 |
| Temperature range (K), max. | 333.62 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 5.86812e+01 |
| Coeff. B | -5.16272e+03 |
| Coeff. C | -6.64398e+00 |
| Coeff. D | 6.01492e-06 |
| Temperature range (K), min. | 167.45 |
| Temperature range (K), max. | 481.20 |

# Sources


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| Activity coefficients at infinite dilution and physicochemical properties for | https://www.doi.org/10.1016/j.jct.2012.08.016 |
| Thermodynamics and selectivity of separation based on activity | https://www.doi.org/10.1016/j.jct.2016.06.028 |
| Separation of binary mixtures | https://www.doi.org/10.1016/j.jct.2017.03.004 |
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| Activity coefficients at infinite dilution for | https://www.doi.org/10.1016/j.jct.2013.08.030 |
| Activity coefficients at infinite dilution for | https://www.doi.org/10.1016/j.jct.2012.01.004 |
| Activity coefficients at infinite dilution of | https://www.doi.org/10.1016/j.jct.2010.12.019 |
| Separation of water/butan-1-ol based | https://www.doi.org/10.1016/j.jct.2017.10.003 |
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| Activity coefficients at infinite dilution | https://www.doi.org/10.1016/j.fluid.2017.12.029 |
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| Activity coefficients at infinite dilution | https://www.doi.org/10.1016/j.fluid.2008.10.008 |
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# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **cpg:** | Ideal gas heat capacity |
| **dm:** | Dipole Moment |
| **gf:** | Standard Gibbs free energy of formation |
| **hcg:** | Heat of Combustion, Gross form |
| **hcn:** | Heat of Combustion, Net Form |
| **hf:** | 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 |
| **rfi:** | Refractive Index |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **srf:** | Surface Tension |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |
| **zc:** | Critical Compressibility |

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