# Pentane, 1-nitro-

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|---|---|
| **Other names:** | 1-Nitropentane |
| | Nitropentane |
| **Inchi:** | InChI=1S/C5H11NO2/c1-2-3-4-5-6(7)8/h2-5H2,1H3 |
| **InchiKey:** | BVALZCVRLDMXOQ-UHFFFAOYSA-N |
| **Formula:** | C5H11NO2 |
| **SMILES:** | CCCCC[N+](=O)[O-] |
| **Mol. weight [g/mol]:** | 117.15 |
| **CAS:** | 628-05-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -3324.00 ± 1.50 | kJ/mol | NIST Webbook |
| gf | 26.77 | kJ/mol | Joback Method |
| hf | -157.29 | kJ/mol | Joback Method |
| hfl | -215.00 ± 1.50 | kJ/mol | NIST Webbook |
| hfus | 20.07 | kJ/mol | Joback Method |
| hvap | 50.30 ± 0.20 | kJ/mol | NIST Webbook |
| log10ws | -2.00 | | Crippen Method |
| logp | 1.453 | | Crippen Method |
| mcvol | 98.730 | ml/mol | McGowan Method |
| pc | 3517.91 | kPa | Joback Method |
| rinpol | 896.00 | | NIST Webbook |
| rinpol | 902.00 | | NIST Webbook |
| rinpol | 941.00 | | NIST Webbook |
| rinpol | 896.00 | | NIST Webbook |
| rinpol | 941.00 | | NIST Webbook |
| rinpol | 902.00 | | NIST Webbook |
| rinpol | 946.04 | | NIST Webbook |
| rinpol | 925.63 | | NIST Webbook |
| rinpol | 947.00 | | NIST Webbook |
| rinpol | 947.00 | | NIST Webbook |
| rinpol | 905.00 | | NIST Webbook |
| rinpol | 910.36 | | NIST Webbook |
| rinpol | 903.31 | | NIST Webbook |
| rinpol | 865.90 | | NIST Webbook |
| rinpol | 910.36 | | NIST Webbook |
| rinpol | 911.95 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 913.83 | | NIST Webbook |
| rinpol | 901.45 | | NIST Webbook |
| rinpol | 902.40 | | NIST Webbook |
| rinpol | 903.31 | | NIST Webbook |
| rinpol | 904.49 | | NIST Webbook |
| rinpol | 905.73 | | NIST Webbook |
| rinpol | 907.12 | | NIST Webbook |
| rinpol | 908.61 | | NIST Webbook |
| rinpol | 865.90 | | NIST Webbook |
| rinpol | 867.00 | | NIST Webbook |
| rinpol | 869.00 | | NIST Webbook |
| rinpol | 855.10 | | NIST Webbook |
| rinpol | 890.00 | | NIST Webbook |
| rinpol | 906.00 | | NIST Webbook |
| rinpol | 906.00 | | NIST Webbook |
| ripol | 1431.00 | | NIST Webbook |
| ripol | 1428.60 | | NIST Webbook |
| ripol | 1414.00 | | NIST Webbook |
| ripol | 1428.60 | | NIST Webbook |
| ripol | 1423.20 | | NIST Webbook |
| ripol | 1418.80 | | NIST Webbook |
| ripol | 1414.00 | | NIST Webbook |
| ripol | 1409.60 | | NIST Webbook |
| ripol | 1405.80 | | NIST Webbook |
| ripol | 1434.50 | | NIST Webbook |
| tb | 445.70 | K | NIST Webbook |
| tc | 670.05 | K | Joback Method |
| tf | 289.72 | K | Joback Method |
| vc | 0.398 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 209.12 | J/mol×K | 465.64 | Joback Method |
| cpg | 219.70 | J/mol×K | 499.71 | Joback Method |
| cpg | 229.76 | J/mol×K | 533.78 | Joback Method |
| cpg | 239.31 | J/mol×K | 567.84 | Joback Method |
| cpg | 248.37 | J/mol×K | 601.91 | Joback Method |
| cpg | 256.96 | J/mol×K | 635.98 | Joback Method |
| cpg | 265.10 | J/mol×K | 670.05 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 348.70 | K | 3.10 | NIST Webbook |

# Sources

**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=C628057&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**rinpol:** Non-polar retention indices
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tbrp:** Boiling point at reduced pressure
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

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