# Cyclopentane, pentyl-

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|---|---|
| **Other names:** | 1-CYCLOPENTYLPENTANE |
| | Cyclopentane, n-pentyl- |
| | PENTYLCYCLOPENTANE |
| | Pentane, 1-cyclopentyl- |
| | n-Amylcyclopentane |
| | n-Pentylcyclopentane |
| **Inchi:** | InChI=1S/C10H20/c1-2-3-4-7-10-8-5-6-9-10/h10H,2-9H2,1H3 |
| **InchiKey:** | HPQURZRDYMUHJI-UHFFFAOYSA-N |
| **Formula:** | C10H20 |
| **SMILES:** | CCCCCC1CCCC1 |
| **Mol. weight [g/mol]:** | 140.27 |
| **CAS:** | 3741-00-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3980 | | KDB |
| chl | -6604.60 ± 1.40 | kJ/mol | NIST Webbook |
| gf | 69.87 | kJ/mol | Joback Method |
| hf | -188.90 ± 1.50 | kJ/mol | NIST Webbook |
| hfus | 15.59 | kJ/mol | Joback Method |
| hvap | 51.00 | kJ/mol | NIST Webbook |
| ie | 9.91 ± 0.05 | eV | NIST Webbook |
| log10ws | -6.08 | | Aqueous Solubility Prediction Method |
| log10ws | -6.08 | | Estimated Solubility Method |
| logp | 3.757 | | Crippen Method |
| mcvol | 140.900 | ml/mol | McGowan Method |
| pc | 2510.00 | kPa | KDB |
| rinpol | 1033.00 | | NIST Webbook |
| rinpol | 1032.00 | | NIST Webbook |
| rinpol | 1032.00 | | NIST Webbook |
| rinpol | 1037.60 | | NIST Webbook |
| rinpol | 1037.00 | | NIST Webbook |
| rinpol | 1041.00 | | NIST Webbook |
| rinpol | 1033.00 | | NIST Webbook |
| rinpol | 1036.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1037.00 | | NIST Webbook |
| rinpol | 1041.00 | | NIST Webbook |
| rinpol | 1033.00 | | NIST Webbook |
| rinpol | 1038.00 | | NIST Webbook |
| rinpol | 1049.00 | | NIST Webbook |
| rinpol | 1033.00 | | NIST Webbook |
| rinpol | 1031.00 | | NIST Webbook |
| rinpol | 1033.00 | | NIST Webbook |
| ripol | 1092.50 | | NIST Webbook |
| ripol | 1113.70 | | NIST Webbook |
| ripol | 1108.30 | | NIST Webbook |
| ripol | 1103.70 | | NIST Webbook |
| ripol | 1107.00 | | NIST Webbook |
| ripol | 1107.00 | | NIST Webbook |
| ripol | 1091.00 | | NIST Webbook |
| ripol | 1095.00 | | NIST Webbook |
| ripol | 1099.00 | | NIST Webbook |
| ripol | 1097.00 | | NIST Webbook |
| ripol | 1099.00 | | NIST Webbook |
| ripol | 1104.00 | | NIST Webbook |
| ripol | 1108.00 | | NIST Webbook |
| ripol | 1114.00 | | NIST Webbook |
| ripol | 1088.00 | | NIST Webbook |
| ripol | 1092.00 | | NIST Webbook |
| ripol | 1097.10 | | NIST Webbook |
| ripol | 1099.10 | | NIST Webbook |
| ripol | 1088.10 | | NIST Webbook |
| tb | 453.80 | K | KDB |
| tb | 453.00 ± 2.00 | K | NIST Webbook |
| tc | 647.50 | K | KDB |
| tf | 190.00 | K | KDB |
| vc | 0.536 | m3/kmol | KDB |
| zc | 0.2501310 | | KDB |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 300.20 | J/mol×K | 443.48 | Joback Method |
| cpg | 318.63 | J/mol×K | 475.04 | Joback Method |
| cpg | 336.18 | J/mol×K | 506.59 | Joback Method |
| cpg | 352.90 | J/mol×K | 538.15 | Joback Method |

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|---|---|---|---|---|
| cpg | 368.79 | J/mol×K | 569.71 | Joback Method |
| cpg | 383.90 | J/mol×K | 601.26 | Joback Method |
| cpg | 398.24 | J/mol×K | 632.82 | Joback Method |
| dvisc | 0.0051754 | Pa×s | 213.36 | Joback Method |
| dvisc | 0.0022556 | Pa×s | 251.71 | Joback Method |
| dvisc | 0.0012245 | Pa×s | 290.07 | Joback Method |
| dvisc | 0.0007667 | Pa×s | 328.42 | Joback Method |
| dvisc | 0.0005294 | Pa×s | 366.77 | Joback Method |
| dvisc | 0.0003921 | Pa×s | 405.13 | Joback Method |
| dvisc | 0.0003059 | Pa×s | 443.48 | Joback Method |
| hvapt | 38.95 | kJ/mol | 453.80 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.47508e+01 |
| Coeff. B | -3.90814e+03 |
| Coeff. C | -6.72950e+01 |
| Temperature range (K), min. | 337.51 |
| Temperature range (K), max. | 481.32 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 1.01985e+02 |
| Coeff. B | -9.59638e+03 |
| Coeff. C | -1.26778e+01 |
| Coeff. D | 6.50164e-06 |
| Temperature range (K), min. | 333.15 |
| Temperature range (K), max. | 647.49 |

# Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3741002&Units=SI |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol583.mol |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=583 |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |
| **zc:** | Critical Compressibility |