# Cyclopentane, (1-methylethyl)-

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|---|---|
| **Other names:** | (1-METHYLETHYL)CYCLOPENTANE |
| | 2-CYCLOPENTYLPROPANE |
| | Cyclopentane, isopropyl- |
| | Isopropylcyclopentane |
| | Propane, 2-cyclopentyl- |
| **Inchi:** | InChI=1S/C8H16/c1-7(2)8-5-3-4-6-8/h7-8H,3-6H2,1-2H3 |
| **InchiKey:** | TVSBRLGQVHJIKT-UHFFFAOYSA-N |
| **Formula:** | C8H16 |
| **SMILES:** | CC(C)C1CCCC1 |
| **Mol. weight [g/mol]:** | 112.21 |
| **CAS:** | 3875-51-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.2400 | | KDB |
| gf | 50.59 | kJ/mol | Joback Method |
| hcg | 5246.32 | kJ/mol | KDB |
| hcn | 4894.444 | kJ/mol | KDB |
| hf | -153.25 | kJ/mol | Joback Method |
| hfus | 6.89 | kJ/mol | Joback Method |
| hvap | 39.48 | kJ/mol | NIST Webbook |
| hvap | 39.40 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 37.90 | kJ/mol | NIST Webbook |
| log10ws | -2.58 | | Crippen Method |
| logp | 2.833 | | Crippen Method |
| mcvol | 112.720 | ml/mol | McGowan Method |
| pc | 3000.00 | kPa | KDB |
| rinpol | 809.20 | | NIST Webbook |
| rinpol | 820.00 | | NIST Webbook |
| rinpol | 830.00 | | NIST Webbook |
| rinpol | 833.00 | | NIST Webbook |
| rinpol | 835.00 | | NIST Webbook |
| rinpol | 838.00 | | NIST Webbook |
| rinpol | 835.00 | | NIST Webbook |
| rinpol | 837.00 | | NIST Webbook |
| rinpol | 812.00 | | NIST Webbook |
| rinpol | 817.00 | | NIST Webbook |

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|---|---|---|
| rinpol | 810.00 | NIST Webbook |
| rinpol | 814.00 | NIST Webbook |
| rinpol | 815.00 | NIST Webbook |
| rinpol | 818.00 | NIST Webbook |
| rinpol | 821.00 | NIST Webbook |
| rinpol | 812.20 | NIST Webbook |
| rinpol | 810.00 | NIST Webbook |
| rinpol | 835.00 | NIST Webbook |
| rinpol | 807.00 | NIST Webbook |
| rinpol | 812.00 | NIST Webbook |
| rinpol | 817.00 | NIST Webbook |
| rinpol | 822.00 | NIST Webbook |
| rinpol | 829.00 | NIST Webbook |
| rinpol | 810.10 | NIST Webbook |
| rinpol | 806.06 | NIST Webbook |
| rinpol | 815.00 | NIST Webbook |
| rinpol | 807.00 | NIST Webbook |
| rinpol | 812.00 | NIST Webbook |
| rinpol | 824.00 | NIST Webbook |
| rinpol | 809.00 | NIST Webbook |
| rinpol | 816.00 | NIST Webbook |
| rinpol | 807.00 | NIST Webbook |
| rinpol | 812.00 | NIST Webbook |
| rinpol | 804.00 | NIST Webbook |
| rinpol | 812.20 | NIST Webbook |
| rinpol | 818.00 | NIST Webbook |
| rinpol | 817.00 | NIST Webbook |
| rinpol | 819.20 | NIST Webbook |
| rinpol | 821.00 | NIST Webbook |
| rinpol | 822.60 | NIST Webbook |
| rinpol | 812.00 | NIST Webbook |
| rinpol | 814.00 | NIST Webbook |
| rinpol | 816.00 | NIST Webbook |
| rinpol | 819.00 | NIST Webbook |
| rinpol | 821.00 | NIST Webbook |
| rinpol | 822.00 | NIST Webbook |
| rinpol | 806.00 | NIST Webbook |
| rinpol | 812.00 | NIST Webbook |
| rinpol | 808.00 | NIST Webbook |
| rinpol | 810.00 | NIST Webbook |
| rinpol | 810.10 | NIST Webbook |
| rinpol | 812.00 | NIST Webbook |
| rinpol | 829.00 | NIST Webbook |
| rinpol | 818.30 | NIST Webbook |

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|---|---|---|---|
| rinpol | 810.80 | | NIST Webbook |
| rinpol | 810.40 | | NIST Webbook |
| rinpol | 812.00 | | NIST Webbook |
| rinpol | 834.10 | | NIST Webbook |
| rinpol | 832.20 | | NIST Webbook |
| rinpol | 817.00 | | NIST Webbook |
| rinpol | 812.10 | | NIST Webbook |
| rinpol | 806.00 | | NIST Webbook |
| rinpol | 817.60 | | NIST Webbook |
| rinpol | 825.00 | | NIST Webbook |
| rinpol | 814.20 | | NIST Webbook |
| tb | 399.57 ± 1.00 | K | NIST Webbook |
| tb | 399.57 ± 1.00 | K | NIST Webbook |
| tb | 399.55 ± 0.50 | K | NIST Webbook |
| tb | 399.70 ± 0.40 | K | NIST Webbook |
| tb | 399.56 ± 0.02 | K | NIST Webbook |
| tb | 399.90 ± 2.00 | K | NIST Webbook |
| tb | 400.10 ± 1.00 | K | NIST Webbook |
| tb | 399.55 ± 0.30 | K | NIST Webbook |
| tb | 399.56 ± 0.01 | K | NIST Webbook |
| tb | 399.60 ± 1.50 | K | NIST Webbook |
| tb | 399.60 ± 2.00 | K | NIST Webbook |
| tb | 399.55 ± 0.20 | K | NIST Webbook |
| tb | 399.60 | K | NIST Webbook |
| tb | 399.60 | K | NIST Webbook |
| tb | 399.60 | K | KDB |
| tb | 399.55 ± 0.30 | K | NIST Webbook |
| tc | 601.00 | K | KDB |
| tf | 160.50 | K | KDB |
| vc | 0.418 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 213.74 | J/mol×K | 397.28 | Joback Method |
| cpg | 230.72 | J/mol×K | 430.18 | Joback Method |
| cpg | 246.88 | J/mol×K | 463.08 | Joback Method |
| cpg | 262.23 | J/mol×K | 495.99 | Joback Method |
| cpg | 276.80 | J/mol×K | 528.89 | Joback Method |
| cpg | 290.62 | J/mol×K | 561.79 | Joback Method |
| cpg | 303.72 | J/mol×K | 594.69 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0013361 | Pa×s | 249.64 | Joback Method |
| dvisc | 0.0027005 | Pa×s | 212.73 | Joback Method |
| dvisc | 0.0073344 | Pa×s | 175.82 | Joback Method |
| dvisc | 0.0007925 | Pa×s | 286.55 | Joback Method |
| dvisc | 0.0005295 | Pa×s | 323.46 | Joback Method |
| dvisc | 0.0003843 | Pa×s | 360.37 | Joback Method |
| dvisc | 0.0002960 | Pa×s | 397.28 | Joback Method |
| hvapt | 33.56 | kJ/mol | 399.60 | NIST Webbook |
| hvapt | 37.90 | kJ/mol | 361.50 | NIST Webbook |
| rfi | 1.42350 | | 298.15 | KDB |
| rhol | 776.00 | kg/m3 | 293.00 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.41783e+01 |
| Coeff. B | -3.34773e+03 |
| Coeff. C | -4.93890e+01 |
| Temperature range (K), min. | 290.39 |
| Temperature range (K), max. | 426.94 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 7.44288e+01 |
| Coeff. B | -7.14690e+03 |
| Coeff. C | -8.79687e+00 |
| Coeff. D | 4.83498e-06 |
| Temperature range (K), min. | 289.15 |
| Temperature range (K), max. | 595.38 |

# Sources

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol481.mol

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3875512&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=481 |
| **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 |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |