# Cyclohexane, 1,2-dimethyl-, trans-

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|---|---|
| **Other names:** | (1R*,2R*)-1,2-dimethylcyclohexane<br>1,2-Dimethyl(trans)-cyclohexane<br>1,2-Dimethylcyclohexane, trans-<br>1,2-trans-Dimethylcyclohexane<br>1,TRANS-2-DIMETHYLCYCLOHEXANE<br>Cyclohexane, trans-1,2-dimethyl-<br>NSC 74158<br>TRANS-1,2-DIMETHYLCYCLOHEXANE<br>t-1,2-Dimethylcyclohexane |
| **Inchi:** | InChI=1S/C8H16/c1-7-5-3-4-6-8(7)2/h7-8H,3-6H2,1-2H3/t7-,8-/m0/s1 |
| **InchiKey:** | KVZJLSYJROEPSQ-YUMQZZPRSA-N |
| **Formula:** | C8H16 |
| **SMILES:** | CC1CCCCC1C |
| **Mol. weight [g/mol]:** | 112.21 |
| **CAS:** | 6876-23-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.2420 | | KDB |
| ap | 321.450 | K | KDB |
| chl | -5216.50 ± 1.80 | kJ/mol | NIST Webbook |
| gf | 34.50 | kJ/mol | KDB |
| hcg | 5216.44 | kJ/mol | KDB |
| hcn | 4864.360 | kJ/mol | KDB |
| hf | -180.10 | kJ/mol | KDB |
| hfus | 9.38 | kJ/mol | Joback Method |
| hvap | 38.40 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 38.35 | kJ/mol | NIST Webbook |
| hvap | 38.30 | kJ/mol | NIST Webbook |
| hvap | 38.41 | kJ/mol | NIST Webbook |
| hvap | 38.40 | kJ/mol | NIST Webbook |
| ie | 10.08 ± 0.03 | eV | NIST Webbook |
| ie | 9.41 | eV | NIST Webbook |
| ie | 10.03 ± 0.05 | eV | NIST Webbook |
| ie | 9.89 ± 0.05 | eV | NIST Webbook |
| log10ws | -2.58 | | Crippen Method |
| logp | 2.833 | | Crippen Method |

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|---|---|---|---|
| mcvol | 112.720 | ml/mol | McGowan Method |
| pc | 2900.00 | kPa | KDB |
| rinpol | 797.70 | | NIST Webbook |
| rinpol | 819.40 | | NIST Webbook |
| rinpol | 820.10 | | NIST Webbook |
| rinpol | 791.80 | | NIST Webbook |
| rinpol | 793.90 | | NIST Webbook |
| rinpol | 796.20 | | NIST Webbook |
| rinpol | 798.40 | | NIST Webbook |
| rinpol | 801.80 | | NIST Webbook |
| rinpol | 797.40 | | NIST Webbook |
| rinpol | 797.80 | | NIST Webbook |
| rinpol | 804.00 | | NIST Webbook |
| rinpol | 794.00 | | NIST Webbook |
| rinpol | 794.00 | | NIST Webbook |
| rinpol | 794.00 | | NIST Webbook |
| rinpol | 818.00 | | NIST Webbook |
| rinpol | 801.50 | | NIST Webbook |
| rinpol | 807.30 | | NIST Webbook |
| rinpol | 812.30 | | NIST Webbook |
| rinpol | 812.50 | | NIST Webbook |
| rinpol | 812.60 | | NIST Webbook |
| rinpol | 807.50 | | NIST Webbook |
| rinpol | 807.60 | | NIST Webbook |
| rinpol | 810.00 | | NIST Webbook |
| rinpol | 810.00 | | NIST Webbook |
| rinpol | 802.00 | | NIST Webbook |
| rinpol | 808.00 | | NIST Webbook |
| rinpol | 799.00 | | NIST Webbook |
| rinpol | 803.00 | | NIST Webbook |
| rinpol | 805.00 | | NIST Webbook |
| rinpol | 808.00 | | NIST Webbook |
| rinpol | 811.00 | | NIST Webbook |
| rinpol | 802.00 | | NIST Webbook |
| rinpol | 799.00 | | NIST Webbook |
| rinpol | 806.00 | | NIST Webbook |
| rinpol | 817.00 | | NIST Webbook |
| rinpol | 802.00 | | NIST Webbook |
| rinpol | 807.00 | | NIST Webbook |
| rinpol | 817.00 | | NIST Webbook |
| rinpol | 802.01 | | NIST Webbook |
| rinpol | 792.00 | | NIST Webbook |
| rinpol | 819.00 | | NIST Webbook |
| rinpol | 792.70 | | NIST Webbook |

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|---|---|---|
| rinpol | 794.00 | NIST Webbook |
| rinpol | 795.70 | NIST Webbook |
| rinpol | 790.99 | NIST Webbook |
| rinpol | 791.42 | NIST Webbook |
| rinpol | 796.70 | NIST Webbook |
| rinpol | 798.00 | NIST Webbook |
| rinpol | 798.40 | NIST Webbook |
| rinpol | 804.80 | NIST Webbook |
| rinpol | 795.10 | NIST Webbook |
| rinpol | 796.70 | NIST Webbook |
| rinpol | 798.00 | NIST Webbook |
| rinpol | 798.40 | NIST Webbook |
| rinpol | 792.78 | NIST Webbook |
| rinpol | 801.10 | NIST Webbook |
| rinpol | 792.00 | NIST Webbook |
| rinpol | 816.00 | NIST Webbook |
| rinpol | 798.00 | NIST Webbook |
| rinpol | 807.00 | NIST Webbook |
| rinpol | 793.00 | NIST Webbook |
| rinpol | 803.80 | NIST Webbook |
| rinpol | 806.80 | NIST Webbook |
| rinpol | 809.20 | NIST Webbook |
| rinpol | 811.20 | NIST Webbook |
| rinpol | 813.00 | NIST Webbook |
| rinpol | 803.00 | NIST Webbook |
| rinpol | 806.00 | NIST Webbook |
| rinpol | 809.00 | NIST Webbook |
| rinpol | 811.00 | NIST Webbook |
| rinpol | 813.00 | NIST Webbook |
| rinpol | 779.00 | NIST Webbook |
| rinpol | 802.00 | NIST Webbook |
| rinpol | 800.00 | NIST Webbook |
| rinpol | 793.00 | NIST Webbook |
| rinpol | 783.00 | NIST Webbook |
| rinpol | 804.00 | NIST Webbook |
| rinpol | 812.00 | NIST Webbook |
| rinpol | 807.00 | NIST Webbook |
| rinpol | 805.00 | NIST Webbook |
| rinpol | 813.00 | NIST Webbook |
| rinpol | 816.00 | NIST Webbook |
| rinpol | 801.80 | NIST Webbook |
| rinpol | 836.60 | NIST Webbook |
| rinpol | 797.50 | NIST Webbook |
| rinpol | 797.80 | NIST Webbook |

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|---|---|---|---|
| rinpol | 797.50 | | NIST Webbook |
| rinpol | 797.40 | | NIST Webbook |
| rinpol | 834.70 | | NIST Webbook |
| rinpol | 828.20 | | NIST Webbook |
| rinpol | 807.70 | | NIST Webbook |
| rinpol | 783.00 | | NIST Webbook |
| rinpol | 837.80 | | NIST Webbook |
| rinpol | 793.00 | | NIST Webbook |
| rinpol | 807.50 | | NIST Webbook |
| rinpol | 793.00 | | NIST Webbook |
| sg | 371.33 | J/mol×K | NIST Webbook |
| sl | 273.22 | J/mol×K | NIST Webbook |
| tb | 396.54 ± 0.30 | K | NIST Webbook |
| tb | 397.00 ± 3.00 | K | NIST Webbook |
| tb | 417.20 ± 0.20 | K | NIST Webbook |
| tb | 396.84 ± 0.30 | K | NIST Webbook |
| tb | 396.85 ± 0.30 | K | NIST Webbook |
| tb | 396.85 ± 0.30 | K | NIST Webbook |
| tb | 396.57 ± 0.20 | K | NIST Webbook |
| tb | 396.70 | K | KDB |
| tb | 396.70 | K | NIST Webbook |
| tb | 396.60 | K | NIST Webbook |
| tb | 397.00 ± 2.00 | K | NIST Webbook |
| tb | 396.56 ± 0.20 | K | NIST Webbook |
| tb | 397.00 ± 2.00 | K | NIST Webbook |
| tb | 396.00 ± 1.50 | K | NIST Webbook |
| tb | 396.56 ± 0.02 | K | NIST Webbook |
| tb | 396.75 ± 0.50 | K | NIST Webbook |
| tb | 396.85 ± 0.30 | K | NIST Webbook |
| tb | 396.54 ± 0.25 | K | NIST Webbook |
| tb | 396.15 ± 0.30 | K | NIST Webbook |
| tc | 596.00 | K | NIST Webbook |
| tc | 596.00 | K | KDB |
| tf | 183.75 ± 0.40 | K | NIST Webbook |
| tf | 184.97 ± 0.04 | K | NIST Webbook |
| tf | 184.45 ± 0.20 | K | NIST Webbook |
| tf | 184.86 ± 0.02 | K | NIST Webbook |
| tf | 184.55 ± 0.50 | K | NIST Webbook |
| tf | 185.00 | K | KDB |
| tf | 184.60 ± 0.50 | K | NIST Webbook |
| tf | 183.55 ± 0.30 | K | NIST Webbook |
| tt | 184.99 ± 0.02 | K | NIST Webbook |
| tt | 184.98 ± 0.05 | K | NIST Webbook |
| tt | 184.99 ± 0.03 | K | NIST Webbook |

| | | | |
|---|---|---|---|
| vc | 0.471 | m3/kmol | KDB |
| zc | 0.2758120 | | KDB |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 307.47 | J/mol×K | 597.67 | Joback Method |
| cpg | 278.84 | J/mol×K | 530.89 | Joback Method |
| cpg | 263.41 | J/mol×K | 497.49 | Joback Method |
| cpg | 247.23 | J/mol×K | 464.10 | Joback Method |
| cpg | 230.28 | J/mol×K | 430.71 | Joback Method |
| cpg | 212.54 | J/mol×K | 397.32 | Joback Method |
| cpg | 293.52 | J/mol×K | 564.28 | Joback Method |
| cpl | 209.41 | J/mol×K | 298.15 | NIST Webbook |
| dvisc | 0.0003324 | Pa×s | 361.61 | Joback Method |
| dvisc | 0.0004419 | Pa×s | 325.90 | Joback Method |
| dvisc | 0.0006303 | Pa×s | 290.19 | Joback Method |
| dvisc | 0.0009932 | Pa×s | 254.48 | Joback Method |
| dvisc | 0.0018154 | Pa×s | 218.77 | Joback Method |
| dvisc | 0.0041986 | Pa×s | 183.06 | Joback Method |
| dvisc | 0.0002631 | Pa×s | 397.32 | Joback Method |
| hfust | 10.50 | kJ/mol | 185.00 | NIST Webbook |
| hfust | 10.49 | kJ/mol | 184.99 | NIST Webbook |
| hfust | 10.50 | kJ/mol | 185.00 | NIST Webbook |
| hvapt | 33.50 ± 0.10 | kJ/mol | 387.00 | NIST Webbook |
| hvapt | 37.00 | kJ/mol | 357.50 | NIST Webbook |
| hvapt | 32.89 | kJ/mol | 396.70 | KDB |
| hvapt | 32.96 | kJ/mol | 396.60 | NIST Webbook |
| hvapt | 34.40 ± 0.10 | kJ/mol | 373.00 | NIST Webbook |
| rfi | 1.42470 | | 298.15 | KDB |
| rhol | 776.00 | kg/m3 | 293.00 | KDB |
| sfust | 56.72 | J/mol×K | 184.99 | NIST Webbook |
| srf | 0.02 | N/m | 293.20 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |

| Equation | ln(Pvp) = A + B/(T + C) |
|---|---|
| Coeff. A | 1.39092e+01 |
| Coeff. B | -3.26861e+03 |
| Coeff. C | -4.48910e+01 |
| Temperature range (K), min. | 284.85 |
| Temperature range (K), max. | 425.06 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 7.15749e+01 |
| Coeff. B | -6.88423e+03 |
| Coeff. C | -8.42118e+00 |
| Coeff. D | 4.99052e-06 |
| Temperature range (K), min. | 184.99 |
| Temperature range (K), max. | 596.15 |

# Sources

| | |
|---|---|
| **Apparatus for the Determination of Water Solubility in Hydrocarbon:** | https://www.doi.org/10.1021/je0502041 |
| **KDB Vapor Pressure Data: Toluene and Alkylcyclohexanes (C6 to C8) from 30 C to 180 C:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=498 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C7-8H15-18 branched alkane solvent:** | https://www.doi.org/10.1016/j.fluid.2006.07.015 |
| **Solubilities of Alkylcyclohexanes in Water from 30 C to 180 C:** | https://www.doi.org/10.1021/je0342567 |
| **KDB:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=498 |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6876239&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Liquid Liquid Equilibria at Three Temperatures (between 280.15 K and 333.15 K) of Binary, Ternary, and Quaternary Systems Involving Monoethylene Glycol, Water, Cyclohexane, para-Xylene, trans- and cis-Dimethylcyclohexane, and trans- and cis-Decahydronaphthalene:** | https://www.doi.org/10.1021/je500625r |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **ap:** | Aniline Point |
| **chl:** | Standard liquid enthalpy of combustion |

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **sfust:** | Entropy of fusion at a given temperature |
| **sg:** | Molar entropy at standard conditions |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **srf:** | Surface Tension |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |
| **zc:** | Critical Compressibility |