

Cyclopentene, 1-methyl-

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|-----------------------------|--|
| Other names: | 1-Cyclopentene, 1-methyl 1-METHYL-1-CYCLOPENTANE 1-Methyl-1-cyclopentene 1-Methylcyclopentene 1-Methylcyclopentene-1 Cyclopentene,1-methyl- |
| Inchi: | InChI=1S/C6H10/c1-6-4-2-3-5-6/h4H,2-3,5H2,1H3 |
| InchiKey: | ATQUFXWBVZUTKO-UHFFFAOYSA-N |
| Formula: | C6H10 |
| SMILES: | CC1=CCCC1 |
| Mol. weight [g/mol]: | 82.14 |
| CAS: | 693-89-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|--------|---------------|
| af | 0.2190 | | KDB |
| affp | 816.50 | kJ/mol | NIST Webbook |
| ap | 266.150 | K | KDB |
| basg | 787.10 | kJ/mol | NIST Webbook |
| chl | -3752.40 ± 0.59 | kJ/mol | NIST Webbook |
| chl | -3753.80 ± 0.54 | kJ/mol | NIST Webbook |
| gf | 64.23 | kJ/mol | Joback Method |
| hcg | 3753.76 | kJ/mol | KDB |
| hcn | 3533.723 | kJ/mol | KDB |
| hf | -4.00 ± 2.00 | kJ/mol | NIST Webbook |
| hf | -3.60 ± 0.75 | kJ/mol | NIST Webbook |
| hf | -2.50 | kJ/mol | NIST Webbook |
| hf | -4.39 | kJ/mol | NIST Webbook |
| hfl | -37.90 ± 0.67 | kJ/mol | NIST Webbook |
| hfl | -36.40 ± 0.63 | kJ/mol | NIST Webbook |
| hfus | 4.99 | kJ/mol | Joback Method |
| hvap | 32.60 ± 0.30 | kJ/mol | NIST Webbook |
| hvap | 34.00 ± 2.00 | kJ/mol | NIST Webbook |
| hvap | 33.90 | kJ/mol | NIST Webbook |
| hvap | 32.60 ± 0.20 | kJ/mol | NIST Webbook |
| ie | 8.62 ± 0.02 | eV | NIST Webbook |
| ie | 8.54 ± 0.01 | eV | NIST Webbook |

| | | | |
|---------|-------------|--------|----------------|
| ie | 8.55 ± 0.01 | eV | NIST Webbook |
| ie | 9.12 ± 0.05 | eV | NIST Webbook |
| ie | 8.60 ± 0.01 | eV | NIST Webbook |
| ie | 8.59 | eV | NIST Webbook |
| log10ws | -2.08 | | Crippen Method |
| logp | 2.117 | | Crippen Method |
| mcvol | 80.240 | ml/mol | McGowan Method |
| pc | 3790.00 | kPa | KDB |
| rinpol | 646.60 | | NIST Webbook |
| rinpol | 662.00 | | NIST Webbook |
| rinpol | 654.00 | | NIST Webbook |
| rinpol | 653.00 | | NIST Webbook |
| rinpol | 643.00 | | NIST Webbook |
| rinpol | 654.00 | | NIST Webbook |
| rinpol | 659.90 | | NIST Webbook |
| rinpol | 644.50 | | NIST Webbook |
| rinpol | 642.00 | | NIST Webbook |
| rinpol | 648.00 | | NIST Webbook |
| rinpol | 647.00 | | NIST Webbook |
| rinpol | 673.00 | | NIST Webbook |
| rinpol | 643.00 | | NIST Webbook |
| rinpol | 647.00 | | NIST Webbook |
| rinpol | 647.00 | | NIST Webbook |
| rinpol | 644.00 | | NIST Webbook |
| rinpol | 654.00 | | NIST Webbook |
| rinpol | 646.00 | | NIST Webbook |
| rinpol | 648.00 | | NIST Webbook |
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| rinpol | 636.00 | | NIST Webbook |
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| rinpol | 643.00 | | NIST Webbook |
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| rinpol | 643.00 | | NIST Webbook |
| rinpol | 645.00 | | NIST Webbook |
| rinpol | 642.00 | | NIST Webbook |
| rinpol | 646.30 | | NIST Webbook |
| rinpol | 641.72 | | NIST Webbook |
| rinpol | 649.00 | | NIST Webbook |
| rinpol | 648.60 | | NIST Webbook |
| rinpol | 675.00 | | NIST Webbook |
| rinpol | 647.00 | | NIST Webbook |
| rinpol | 647.00 | | NIST Webbook |
| rinpol | 660.00 | | NIST Webbook |
| rinpol | 650.00 | | NIST Webbook |

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| rinpol | 648.00 | NIST Webbook |
| rinpol | 645.00 | NIST Webbook |
| rinpol | 642.00 | NIST Webbook |
| rinpol | 649.00 | NIST Webbook |
| rinpol | 647.00 | NIST Webbook |
| rinpol | 644.00 | NIST Webbook |
| rinpol | 654.00 | NIST Webbook |
| rinpol | 654.00 | NIST Webbook |
| rinpol | 651.00 | NIST Webbook |
| rinpol | 675.00 | NIST Webbook |
| rinpol | 663.10 | NIST Webbook |
| rinpol | 659.90 | NIST Webbook |
| rinpol | 649.00 | NIST Webbook |
| rinpol | 649.00 | NIST Webbook |
| rinpol | 660.00 | NIST Webbook |
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| rinpol | 646.50 | NIST Webbook |
| rinpol | 643.80 | NIST Webbook |
| rinpol | 646.10 | NIST Webbook |
| rinpol | 650.00 | NIST Webbook |
| rinpol | 642.00 | NIST Webbook |
| rinpol | 641.00 | NIST Webbook |
| rinpol | 645.00 | NIST Webbook |
| rinpol | 648.00 | NIST Webbook |
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| rinpol | 644.55 | NIST Webbook |
| rinpol | 651.00 | NIST Webbook |
| rinpol | 643.00 | NIST Webbook |
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| rinpol | 650.00 | NIST Webbook |
| rinpol | 648.00 | NIST Webbook |
| rinpol | 644.00 | NIST Webbook |
| rinpol | 647.00 | NIST Webbook |
| rinpol | 673.00 | NIST Webbook |
| rinpol | 677.00 | NIST Webbook |
| rinpol | 644.50 | NIST Webbook |
| rinpol | 650.00 | NIST Webbook |
| rinpol | 674.00 | NIST Webbook |
| ripol | 792.00 | NIST Webbook |
| ripol | 786.00 | NIST Webbook |
| ripol | 792.00 | NIST Webbook |

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|-------|---------------|----------------------|---------------|
| ripol | 791.90 | | NIST Webbook |
| ripol | 781.50 | | NIST Webbook |
| ripol | 786.00 | | NIST Webbook |
| ripol | 791.90 | | NIST Webbook |
| ripol | 781.50 | | NIST Webbook |
| ripol | 786.00 | | NIST Webbook |
| ripol | 792.00 | | NIST Webbook |
| ripol | 781.50 | | NIST Webbook |
| ripol | 782.00 | | NIST Webbook |
| tb | 349.00 ± 3.00 | K | NIST Webbook |
| tb | 348.00 ± 3.00 | K | NIST Webbook |
| tb | 348.35 ± 0.50 | K | NIST Webbook |
| tb | 349.00 ± 0.40 | K | NIST Webbook |
| tb | 348.20 ± 2.00 | K | NIST Webbook |
| tb | 347.70 ± 2.00 | K | NIST Webbook |
| tb | 348.75 ± 0.30 | K | NIST Webbook |
| tb | 347.90 ± 2.00 | K | NIST Webbook |
| tb | 348.64 ± 0.30 | K | NIST Webbook |
| tb | 348.00 ± 3.00 | K | NIST Webbook |
| tb | 348.90 ± 0.20 | K | NIST Webbook |
| tb | 348.90 ± 2.00 | K | NIST Webbook |
| tb | 351.00 ± 1.00 | K | NIST Webbook |
| tb | 349.00 ± 3.00 | K | NIST Webbook |
| tb | 348.60 ± 0.40 | K | NIST Webbook |
| tb | 348.70 | K | NIST Webbook |
| tb | 349.00 | K | KDB |
| tb | 348.75 ± 0.30 | K | NIST Webbook |
| tb | 348.90 ± 2.00 | K | NIST Webbook |
| tb | 348.95 ± 0.60 | K | NIST Webbook |
| tb | 347.00 ± 3.00 | K | NIST Webbook |
| tb | 348.95 ± 0.50 | K | NIST Webbook |
| tb | 349.00 ± 0.20 | K | NIST Webbook |
| tb | 348.90 ± 2.00 | K | NIST Webbook |
| tb | 348.65 ± 0.50 | K | NIST Webbook |
| tb | 349.00 ± 3.00 | K | NIST Webbook |
| tb | 347.00 ± 6.00 | K | NIST Webbook |
| tb | 343.00 ± 5.00 | K | NIST Webbook |
| tb | 348.00 ± 3.00 | K | NIST Webbook |
| tc | 542.00 | K | KDB |
| tf | 146.00 | K | KDB |
| vc | 0.299 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 190.05 | J/molxK | 560.35 | Joback Method |
| cpg | 181.05 | J/molxK | 527.08 | Joback Method |
| cpg | 127.75 | J/molxK | 360.77 | Joback Method |
| cpg | 139.60 | J/molxK | 394.03 | Joback Method |
| cpg | 150.83 | J/molxK | 427.30 | Joback Method |
| cpg | 161.46 | J/molxK | 460.56 | Joback Method |
| cpg | 171.53 | J/molxK | 493.82 | Joback Method |
| cpl | 153.10 | J/molxK | 298.15 | NIST Webbook |
| dvisc | 0.0002644 | Paxs | 360.77 | Joback Method |
| dvisc | 0.0003282 | Paxs | 331.61 | Joback Method |
| dvisc | 0.0026779 | Paxs | 185.80 | Joback Method |
| dvisc | 0.0014013 | Paxs | 214.96 | Joback Method |
| dvisc | 0.0008560 | Paxs | 244.12 | Joback Method |
| dvisc | 0.0005809 | Paxs | 273.28 | Joback Method |
| dvisc | 0.0004248 | Paxs | 302.45 | Joback Method |
| hvapt | 33.40 | kJ/mol | 335.50 | NIST Webbook |
| rfi | 1.42940 | | 298.15 | KDB |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 345.20 | K | 101.00 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.39480e+01 |
| Coeff. B | -2.84120e+03 |
| Coeff. C | -4.44650e+01 |
| Temperature range (K), min. | 252.45 |

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|-----------------------------|--------|
| Temperature range (K), max. | 373.44 |
|-----------------------------|--------|

| Information | Value |
|-----------------------------|--|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A | 6.71668e+01 |
| Coeff. B | -5.97528e+03 |
| Coeff. C | -7.87810e+00 |
| Coeff. D | 5.76113e-06 |
| Temperature range (K), min. | 268.15 |
| Temperature range (K), max. | 541.99 |

Sources

| | |
|---|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C693890&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.thermo.com/research/kdb/hcprop/showprop.php?cmpid=611 |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemed.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| KDB: | https://www.thermo.com/files/research/kdb/mol/mol611.mol |

Legend

| | |
|---------------|--|
| af: | Acentric Factor |
| affp: | Proton affinity |
| ap: | Aniline Point |
| basg: | Gas basicity |
| 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 |

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| hfl: | Liquid phase 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 |
| mcpvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| pvap: | Vapor pressure |
| rfi: | Refractive Index |
| 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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