

# 2-Pentene, 4-methyl-, (Z)-

|                      |                                                                                                                                                                                                                                                                |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (Z)-(CH3)2CHCH=CHCH3<br>(Z)-4-METHYL-2-PENTENE<br>2-Pentene, 4-methyl-cis-<br>4-METHYL-CIS-2-PENTENE<br>4-Methyl-2-cis-pentene<br>4-Methyl-2-pentene<br>4-Methyl-2-pentene, cis<br>4-Methylpentene-2, cis-<br>CIS-4-METHYL-2-PENTENE<br>cis-4-methylpent-2-ene |
| Inchi:               | InChI=1S/C6H12/c1-4-5-6(2)3/h4-6H,1-3H3/b5-4-                                                                                                                                                                                                                  |
| InchiKey:            | LGAQJENWWYGFSN-PLNGDYQASA-N                                                                                                                                                                                                                                    |
| Formula:             | C6H12                                                                                                                                                                                                                                                          |
| SMILES:              | CC=CC(C)C                                                                                                                                                                                                                                                      |
| Mol. weight [g/mol]: | 84.16                                                                                                                                                                                                                                                          |
| CAS:                 | 691-38-3                                                                                                                                                                                                                                                       |

## Physical Properties

| Property code | Value          | Unit   | Source         |
|---------------|----------------|--------|----------------|
| af            | 0.2900         |        | KDB            |
| gf            | 82.19          | kJ/mol | KDB            |
| hcg           | 3989.11        | kJ/mol | KDB            |
| hcn           | 3725.015       | kJ/mol | KDB            |
| hf            | -57.48         | kJ/mol | KDB            |
| hfus          | 7.98           | kJ/mol | Joback Method  |
| hvap          | 29.50          | kJ/mol | NIST Webbook   |
| hvap          | 29.50          | kJ/mol | NIST Webbook   |
| hvap          | 29.50          | kJ/mol | NIST Webbook   |
| ie            | 8.98 ± 0.02    | eV     | NIST Webbook   |
| ie            | 8.98 ± 0.01    | eV     | NIST Webbook   |
| ie            | 8.98 ± 0.01    | eV     | NIST Webbook   |
| log10ws       | -1.95          |        | Crippen Method |
| logp          | 2.219          |        | Crippen Method |
| mcvol         | 91.100         | ml/mol | McGowan Method |
| nfpaf         | %!d(float64=3) |        | KDB            |
| nfpah         | %!d(float64=1) |        | KDB            |
| pc            | 3040.00        | kPa    | KDB            |

|        |        |              |
|--------|--------|--------------|
| rinpol | 566.00 | NIST Webbook |
| rinpol | 557.00 | NIST Webbook |
| rinpol | 559.00 | NIST Webbook |
| rinpol | 570.00 | NIST Webbook |
| rinpol | 569.00 | NIST Webbook |
| rinpol | 557.00 | NIST Webbook |
| rinpol | 566.00 | NIST Webbook |
| rinpol | 567.50 | NIST Webbook |
| rinpol | 558.00 | NIST Webbook |
| rinpol | 556.20 | NIST Webbook |
| rinpol | 556.00 | NIST Webbook |
| rinpol | 560.70 | NIST Webbook |
| rinpol | 561.00 | NIST Webbook |
| rinpol | 555.90 | NIST Webbook |
| rinpol | 567.50 | NIST Webbook |
| rinpol | 555.50 | NIST Webbook |
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| rinpol | 565.60 | NIST Webbook |
| rinpol | 566.10 | NIST Webbook |
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| rinpol | 560.70 | NIST Webbook |
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| rinpol | 557.00 | NIST Webbook |
| rinpol | 555.36 | NIST Webbook |
| rinpol | 561.00 | NIST Webbook |
| rinpol | 556.00 | NIST Webbook |
| rinpol | 556.00 | NIST Webbook |
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| rinpol | 558.00 | NIST Webbook |
| rinpol | 556.00 | NIST Webbook |

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|--------|---------------|---------|-----------------------------------------------------------------------------------|
| rinpol | 561.00        |         | NIST Webbook                                                                      |
| rinpol | 560.00        |         | NIST Webbook                                                                      |
| rinpol | 558.00        |         | NIST Webbook                                                                      |
| rinpol | 571.20        |         | NIST Webbook                                                                      |
| rinpol | 565.90        |         | NIST Webbook                                                                      |
| rinpol | 559.00        |         | NIST Webbook                                                                      |
| rinpol | 555.90        |         | NIST Webbook                                                                      |
| rinpol | 553.00        |         | NIST Webbook                                                                      |
| rinpol | 556.00        |         | NIST Webbook                                                                      |
| rinpol | 572.00        |         | NIST Webbook                                                                      |
| rinpol | 556.00        |         | NIST Webbook                                                                      |
| rinpol | 570.00        |         | NIST Webbook                                                                      |
| tb     | 329.60        | K       | KDB                                                                               |
| tb     | 327.85 ± 0.60 | K       | NIST Webbook                                                                      |
| tb     | 331.20 ± 2.00 | K       | NIST Webbook                                                                      |
| tb     | 329.15 ± 2.00 | K       | NIST Webbook                                                                      |
| tb     | 328.15 ± 4.00 | K       | NIST Webbook                                                                      |
| tb     | 327.95 ± 1.50 | K       | NIST Webbook                                                                      |
| tb     | 327.85 ± 1.00 | K       | NIST Webbook                                                                      |
| tb     | 329.15 ± 1.50 | K       | NIST Webbook                                                                      |
| tb     | 329.65 ± 1.00 | K       | NIST Webbook                                                                      |
| tb     | 329.55 ± 0.50 | K       | NIST Webbook                                                                      |
| tb     | 329.56 ± 0.50 | K       | NIST Webbook                                                                      |
| tb     | 329.45 ± 0.50 | K       | NIST Webbook                                                                      |
| tb     | 329.50        | K       | NIST Webbook                                                                      |
| tb     | 330.50 ± 0.50 | K       | NIST Webbook                                                                      |
| tb     | 330.70        | K       | NIST Webbook                                                                      |
| tc     | 490.00        | K       | KDB                                                                               |
| tc     | 496.30        | K       | Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons |
| tf     | 139.00        | K       | KDB                                                                               |
| vc     | 0.360         | m3/kmol | KDB                                                                               |
| zc     | 0.2686230     |         | KDB                                                                               |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 202.31 | J/mol×K | 517.01          | Joback Method |
| cpg           | 144.81 | J/mol×K | 340.40          | Joback Method |
| cpg           | 155.51 | J/mol×K | 369.83          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 165.74    | J/mol×K | 399.27 | Joback Method |
| cpg   | 175.52    | J/mol×K | 428.70 | Joback Method |
| cpg   | 184.87    | J/mol×K | 458.14 | Joback Method |
| cpg   | 193.79    | J/mol×K | 487.57 | Joback Method |
| dvisc | 0.0001822 | Pa×s    | 340.40 | Joback Method |
| dvisc | 0.0086948 | Pa×s    | 137.30 | Joback Method |
| dvisc | 0.0024144 | Pa×s    | 171.15 | Joback Method |
| dvisc | 0.0010236 | Pa×s    | 205.00 | Joback Method |
| dvisc | 0.0005535 | Pa×s    | 238.85 | Joback Method |
| dvisc | 0.0003486 | Pa×s    | 272.70 | Joback Method |
| dvisc | 0.0002432 | Pa×s    | 306.55 | Joback Method |
| hvapt | 30.80     | kJ/mol  | 298.50 | NIST Webbook  |
| hvapt | 27.57     | kJ/mol  | 329.60 | KDB           |
| rfi   | 1.38498   |         | 298.15 | KDB           |
| rhoI  | 669.00    | kg/m3   | 293.00 | KDB           |
| srf   | 0.02      | N/m     | 298.20 | KDB           |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.40679e+01                   |
| Coeff. B                    | -2.77368e+03                  |
| Coeff. C                    | -3.60040e+01                  |
| Temperature range (K), min. | 237.28                        |
| Temperature range (K), max. | 352.77                        |

| Information                 | Value                                                  |
|-----------------------------|--------------------------------------------------------|
| Property code               | pvap                                                   |
| Equation                    | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A                    | 7.59746e+01                                            |
| Coeff. B                    | -5.96255e+03                                           |
| Coeff. C                    | -9.34598e+00                                           |
| Coeff. D                    | 8.49625e-06                                            |
| Temperature range (K), min. | 138.30                                                 |
| Temperature range (K), max. | 499.00                                                 |

# Sources

|                                                                                           |                                                                                                                                                                                         |
|-------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b>                                                                    | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| <b>NIST Webbook:</b>                                                                      | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C691383&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C691383&amp;Units=SI</a>                                               |
| <b>Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:</b> | <a href="https://www.doi.org/10.1021/je0341357">https://www.doi.org/10.1021/je0341357</a>                                                                                               |
| <b>Crippen Method:</b>                                                                    | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                                                               |
| <b>KDB:</b>                                                                               | <a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=207">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=207</a>                                       |
| <b>The Yaws Handbook of Vapor Pressure:</b>                                               | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| <b>KDB Vapor Pressure Data:</b>                                                           | <a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=207">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=207</a>                                       |
| <b>Joback Method:</b>                                                                     | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| <b>McGowan Method:</b>                                                                    | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hcg:</b>     | Heat of Combustion, Gross form                  |
| <b>hcn:</b>     | Heat of Combustion, Net Form                    |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>nfpaf:</b>   | NFPA Fire Rating                                |
| <b>nfpah:</b>   | NFPA Health Rating                              |
| <b>pc:</b>      | Critical Pressure                               |
| <b>pvap:</b>    | Vapor pressure                                  |
| <b>rfi:</b>     | Refractive Index                                |
| <b>rho:</b>     | Liquid Density                                  |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>srf:</b>     | Surface Tension                                 |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |

**vc:** Critical Volume  
**zc:** Critical Compressibility

Latest version available from:

<https://www.chemeo.com/cid/38-574-3/2-Pentene-4-methyl-Z.pdf>

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