

# 2,3-Pentadiene, 2,4-dimethyl-

|                      |                                                                                                                                                           |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (CH3)2C=C=C(CH3)2<br>1,1,3,3-Tetramethylallene<br>2,4-Dimethyl-2,3-pentadiene<br>2,4-dimethylpenta-2,3-diene<br>Allene, tetramethyl-<br>Tetramethylallene |
| Inchi:               | InChI=1S/C7H12/c1-6(2)5-7(3)4/h1-4H3                                                                                                                      |
| InchiKey:            | DZSNJASVIURWOG-UHFFFAOYSA-N                                                                                                                               |
| Formula:             | C7H12                                                                                                                                                     |
| SMILES:              | CC(C)=C=C(C)C                                                                                                                                             |
| Mol. weight [g/mol]: | 96.17                                                                                                                                                     |
| CAS:                 | 1000-87-9                                                                                                                                                 |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 199.46        | kJ/mol  | Joback Method  |
| hf            | 72.61         | kJ/mol  | Joback Method  |
| hfus          | 13.60         | kJ/mol  | Joback Method  |
| hvap          | 31.73         | kJ/mol  | Joback Method  |
| ie            | 8.47          | eV      | NIST Webbook   |
| ie            | 8.53          | eV      | NIST Webbook   |
| log10ws       | -2.48         |         | Crippen Method |
| logp          | 2.518         |         | Crippen Method |
| mcvol         | 100.890       | ml/mol  | McGowan Method |
| pc            | 3318.18       | kPa     | Joback Method  |
| tb            | 356.00 ± 4.00 | K       | NIST Webbook   |
| tb            | 356.00 ± 3.00 | K       | NIST Webbook   |
| tc            | 558.45        | K       | Joback Method  |
| tf            | 142.16        | K       | Joback Method  |
| vc            | 0.390         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
|---------------|-------|------|-----------------|--------|

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 172.58 | J/mol×K | 366.75 | Joback Method |
| cpg | 183.53 | J/mol×K | 398.70 | Joback Method |
| cpg | 194.04 | J/mol×K | 430.65 | Joback Method |
| cpg | 204.12 | J/mol×K | 462.60 | Joback Method |
| cpg | 213.78 | J/mol×K | 494.55 | Joback Method |
| cpg | 223.03 | J/mol×K | 526.50 | Joback Method |
| cpg | 231.89 | J/mol×K | 558.45 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.58583e+01                   |
| Coeff. B                    | -3.54255e+03                  |
| Coeff. C                    | -4.08270e+01                  |
| Temperature range (K), min. | 268.34                        |
| Temperature range (K), max. | 376.71                        |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1000879&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1000879&amp;Units=SI</a>                                             |
| The Yaws Handbook of Vapor Pressure: | <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> |
| Crippen Method:                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                                                               |
| Crippen Method:                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| Joback Method:                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| McGowan Method:                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |

## Legend

|       |                                                 |
|-------|-------------------------------------------------|
| cpg:  | Ideal gas heat capacity                         |
| 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 |

|                 |                                     |
|-----------------|-------------------------------------|
| <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>pc:</b>      | Critical Pressure                   |
| <b>pvap:</b>    | Vapor pressure                      |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tc:</b>      | Critical Temperature                |
| <b>tf:</b>      | Normal melting (fusion) point       |
| <b>vc:</b>      | Critical Volume                     |

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