# 1,3-Pentadiene, 2,4-dimethyl-

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|---|---|
| **Other names:** | (CH3)2C=CHC(CH3)=CH2 |
| | 1,1,3-TRIMETHYLBUTADIENE |
| | 2,4-Dimethyl-1,3-pentadiene |
| | 2,4-dimethylpenta-1,3-diene |
| **Inchi:** | InChI=1S/C7H12/c1-6(2)5-7(3)4/h5H,1H2,2-4H3 |
| **InchiKey:** | CMSUNVGIWAFNBG-UHFFFAOYSA-N |
| **Formula:** | C7H12 |
| **SMILES:** | C=C(C)C=C(C)C |
| **Mol. weight [g/mol]:** | 96.17 |
| **CAS:** | 1000-86-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 886.50 | kJ/mol | NIST Webbook |
| basg | 857.60 | kJ/mol | NIST Webbook |
| gf | 159.02 | kJ/mol | Joback Method |
| hf | 35.26 | kJ/mol | Joback Method |
| hfus | 10.19 | kJ/mol | Joback Method |
| hvap | 30.62 | kJ/mol | Joback Method |
| log10ws | -2.46 | | Crippen Method |
| logp | 2.529 | | Crippen Method |
| mcvol | 100.890 | ml/mol | McGowan Method |
| pc | 3135.00 | kPa | Joback Method |
| rinpol | 700.00 | | NIST Webbook |
| rinpol | 686.00 | | NIST Webbook |
| rinpol | 687.00 | | NIST Webbook |
| rinpol | 688.00 | | NIST Webbook |
| rinpol | 688.00 | | NIST Webbook |
| rinpol | 698.00 | | NIST Webbook |
| rinpol | 700.00 | | NIST Webbook |
| rinpol | 698.00 | | NIST Webbook |
| rinpol | 687.00 | | NIST Webbook |
| rinpol | 698.00 | | NIST Webbook |
| tb | 360.16 | K | Joback Method |
| tc | 543.50 | K | Joback Method |
| tf | 157.15 ± 1.00 | K | NIST Webbook |
| tf | 159.15 ± 5.00 | K | NIST Webbook |

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|---|---|---|---|
| tf | 157.15 ± 0.50 | K | NIST Webbook |
| tf | 157.15 ± 0.40 | K | NIST Webbook |
| tf | 157.20 ± 0.50 | K | NIST Webbook |
| vc | 0.391 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 166.61 | J/mol×K | 360.16 | Joback Method |
| cpg | 178.12 | J/mol×K | 390.72 | Joback Method |
| cpg | 189.05 | J/mol×K | 421.27 | Joback Method |
| cpg | 199.45 | J/mol×K | 451.83 | Joback Method |
| cpg | 209.32 | J/mol×K | 482.38 | Joback Method |
| cpg | 218.70 | J/mol×K | 512.94 | Joback Method |
| cpg | 227.61 | J/mol×K | 543.50 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.55174e+01 |
| Coeff. B | -3.52699e+03 |
| Coeff. C | -4.29950e+01 |
| Temperature range (K), min. | 274.58 |
| Temperature range (K), max. | 388.58 |

# Sources

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1000868&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**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

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol390.mol

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |