# 2-Methyl-2-heptene

**Other names:** 2-Heptene, 2-methyl-
2-Methylhept-2-ene
**Inchi:** InChI=1S/C8H16/c1-4-5-6-7-8(2)3/h7H,4-6H2,1-3H3
**InchiKey:** WEPNJTDVIIKRIK-UHFFFAOYSA-N
**Formula:** C8H16
**SMILES:** CCCCC=C(C)C
**Mol. weight [g/mol]:** 112.21
**CAS:** 627-97-4

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 88.15 | kJ/mol | Joback Method |
| hf | -101.02 | kJ/mol | Joback Method |
| hfus | 15.37 | kJ/mol | Joback Method |
| hvap | 39.70 | kJ/mol | NIST Webbook |
| log10ws | -3.02 | | Crippen Method |
| logp | 3.143 | | Crippen Method |
| mcvol | 119.280 | ml/mol | McGowan Method |
| pc | 2687.42 | kPa | Joback Method |
| rinpol | 800.00 | | NIST Webbook |
| rinpol | 791.00 | | NIST Webbook |
| rinpol | 789.50 | | NIST Webbook |
| rinpol | 800.00 | | NIST Webbook |
| rinpol | 800.00 | | NIST Webbook |
| rinpol | 786.00 | | NIST Webbook |
| rinpol | 770.00 | | NIST Webbook |
| rinpol | 796.00 | | NIST Webbook |
| rinpol | 770.00 | | NIST Webbook |
| rinpol | 789.50 | | NIST Webbook |
| rinpol | 786.00 | | NIST Webbook |
| rinpol | 787.00 | | NIST Webbook |
| rinpol | 789.60 | | NIST Webbook |
| rinpol | 800.20 | | NIST Webbook |
| rinpol | 789.50 | | NIST Webbook |
| rinpol | 786.00 | | NIST Webbook |
| tb | 395.75 ± 0.50 | K | NIST Webbook |
| tb | 395.85 ± 0.40 | K | NIST Webbook |

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|---|---|---|---|
| tb | 398.35 ± 0.60 | K | NIST Webbook |
| tb | 394.85 ± 0.70 | K | NIST Webbook |
| tb | 394.65 ± 1.00 | K | NIST Webbook |
| tb | 393.65 ± 2.00 | K | NIST Webbook |
| tb | 394.75 ± 0.70 | K | NIST Webbook |
| tb | 395.80 | K | NIST Webbook |
| tb | 395.75 ± 0.60 | K | NIST Webbook |
| tb | 395.77 ± 0.20 | K | NIST Webbook |
| tb | 396.02 ± 0.20 | K | NIST Webbook |
| tb | 395.83 ± 0.20 | K | NIST Webbook |
| tc | 568.90 | K | Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons |
| tf | 151.00 ± 0.02 | K | NIST Webbook |
| tf | 150.98 ± 0.06 | K | NIST Webbook |
| tf | 150.98 ± 0.06 | K | NIST Webbook |
| vc | 0.465 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 278.15 | J/mol×K | 532.54 | Joback Method |
| cpg | 218.03 | J/mol×K | 386.48 | Joback Method |
| cpg | 231.15 | J/mol×K | 415.69 | Joback Method |
| cpg | 243.70 | J/mol×K | 444.90 | Joback Method |
| cpg | 255.70 | J/mol×K | 474.11 | Joback Method |
| cpg | 267.18 | J/mol×K | 503.32 | Joback Method |
| cpg | 288.64 | J/mol×K | 561.75 | Joback Method |
| hvapt | 41.20 | kJ/mol | 326.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.42166e+01 |
| Coeff. B | -3.33544e+03 |
| Coeff. C | -4.84960e+01 |

| | |
|---|---|
| Temperature range (K), min. | 287.96 |
| Temperature range (K), max. | 423.05 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 9.49092e+01 |
| Coeff. B | -7.89919e+03 |
| Coeff. C | -1.19986e+01 |
| Coeff. D | 9.12422e-06 |
| Temperature range (K), min. | 288.15 |
| Temperature range (K), max. | 423.15 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C627974&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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 |
| **Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:** | https://www.doi.org/10.1021/je0341357 |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=261 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol261.mol |

# Legend

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|---|---|
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |