# Heptane, 4-methyl-

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|---|---|
| **Other names:** | (n-C3H7)2CHCH3 |
| | 4-Methylheptane |
| **Inchi:** | InChI=1S/C8H18/c1-4-6-8(3)7-5-2/h8H,4-7H2,1-3H3 |
| **InchiKey:** | CHBAWFGIXDBEBT-UHFFFAOYSA-N |
| **Formula:** | C8H18 |
| **SMILES:** | CCCC(C)CCC |
| **Mol. weight [g/mol]:** | 114.23 |
| **CAS:** | 589-53-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3710 | | KDB |
| ap | 344.750 | K | KDB |
| chl | -5468.90 ± 1.00 | kJ/mol | NIST Webbook |
| gf | 16.75 | kJ/mol | KDB |
| hcg | 5468.86 | kJ/mol | KDB |
| hcn | 5072.724 | kJ/mol | KDB |
| hf | -212.20 | kJ/mol | KDB |
| hf | -212.10 ± 1.20 | kJ/mol | NIST Webbook |
| hfl | -251.80 ± 1.20 | kJ/mol | NIST Webbook |
| hfus | 12.95 | kJ/mol | Joback Method |
| hvap | 39.70 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 39.70 | kJ/mol | NIST Webbook |
| hvap | 39.70 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 39.67 | kJ/mol | NIST Webbook |
| hvap | 39.75 | kJ/mol | NIST Webbook |
| hvap | 33.80 ± 0.08 | kJ/mol | NIST Webbook |
| log10ws | -2.93 | | Crippen Method |
| logp | 3.223 | | Crippen Method |
| mcvol | 123.580 | ml/mol | McGowan Method |
| pc | 2540.00 | kPa | KDB |
| pc | 2540.00 ± 40.00 | kPa | NIST Webbook |
| pc | 2541.90 ± 40.53 | kPa | NIST Webbook |
| rhoc | 239.88 ± 4.57 | kg/m3 | NIST Webbook |
| rhoc | 239.88 ± 4.57 | kg/m3 | NIST Webbook |
| rinpol | 767.00 | | NIST Webbook |
| rinpol | 775.00 | | NIST Webbook |

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|---|---|---|
| rinpol | 770.00 | NIST Webbook |
| rinpol | 770.00 | NIST Webbook |
| rinpol | 764.00 | NIST Webbook |
| rinpol | 766.00 | NIST Webbook |
| rinpol | 767.00 | NIST Webbook |
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| rinpol | 766.00 | NIST Webbook |
| rinpol | 767.00 | NIST Webbook |
| rinpol | 775.00 | NIST Webbook |
| rinpol | 777.73 | NIST Webbook |
| rinpol | 768.40 | NIST Webbook |
| rinpol | 765.60 | NIST Webbook |
| rinpol | 767.00 | NIST Webbook |
| rinpol | 767.00 | NIST Webbook |
| rinpol | 769.00 | NIST Webbook |
| rinpol | 767.00 | NIST Webbook |
| rinpol | 768.00 | NIST Webbook |
| rinpol | 766.80 | NIST Webbook |
| rinpol | 767.16 | NIST Webbook |
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| rinpol | 767.20 | NIST Webbook |
| rinpol | 762.00 | NIST Webbook |
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| rinpol | 767.60 | NIST Webbook |
| rinpol | 767.80 | NIST Webbook |
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| rinpol | 768.00 | NIST Webbook |
| rinpol | 767.00 | NIST Webbook |
| rinpol | 757.00 | NIST Webbook |
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| rinpol | 771.00 | NIST Webbook |
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| rinpol | 770.00 | NIST Webbook |
| rinpol | 768.40 | NIST Webbook |
| rinpol | 762.88 | NIST Webbook |
| rinpol | 763.26 | NIST Webbook |
| rinpol | 760.40 | NIST Webbook |
| rinpol | 764.60 | NIST Webbook |
| rinpol | 765.60 | NIST Webbook |
| rinpol | 762.50 | NIST Webbook |
| rinpol | 762.50 | NIST Webbook |
| rinpol | 763.78 | NIST Webbook |
| rinpol | 763.91 | NIST Webbook |
| rinpol | 767.00 | NIST Webbook |
| rinpol | 764.38 | NIST Webbook |
| rinpol | 764.57 | NIST Webbook |
| rinpol | 765.00 | NIST Webbook |
| rinpol | 767.70 | NIST Webbook |
| rinpol | 766.80 | NIST Webbook |
| rinpol | 768.50 | NIST Webbook |
| rinpol | 767.75 | NIST Webbook |
| rinpol | 768.05 | NIST Webbook |
| rinpol | 768.28 | NIST Webbook |
| rinpol | 767.16 | NIST Webbook |
| rinpol | 767.53 | NIST Webbook |
| rinpol | 767.77 | NIST Webbook |
| rinpol | 762.00 | NIST Webbook |
| rinpol | 777.73 | NIST Webbook |
| rinpol | 756.00 | NIST Webbook |
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| rinpol | 759.00 | NIST Webbook |
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| rinpol | 765.00 | | NIST Webbook |
| rinpol | 768.00 | | NIST Webbook |
| rinpol | 769.00 | | NIST Webbook |
| rinpol | 768.00 | | NIST Webbook |
| ripol | 764.00 | | NIST Webbook |
| ripol | 790.00 | | NIST Webbook |
| ripol | 768.00 | | NIST Webbook |
| tb | 390.90 | K | NIST Webbook |
| tb | 390.87 | K | KDB |
| tb | 391.15 ± 2.00 | K | NIST Webbook |
| tb | 391.15 ± 1.00 | K | NIST Webbook |
| tb | 391.15 ± 0.20 | K | NIST Webbook |
| tb | 391.15 ± 0.40 | K | NIST Webbook |
| tb | 391.15 ± 0.60 | K | NIST Webbook |
| tb | 390.65 ± 0.30 | K | NIST Webbook |
| tb | 390.65 ± 0.30 | K | NIST Webbook |
| tb | 390.65 ± 0.60 | K | NIST Webbook |
| tb | 390.86 ± 0.20 | K | NIST Webbook |
| tb | 391.15 ± 2.00 | K | NIST Webbook |
| tb | 390.75 ± 0.50 | K | NIST Webbook |
| tb | 390.76 ± 0.30 | K | NIST Webbook |
| tb | 390.85 ± 0.01 | K | NIST Webbook |
| tb | 390.78 ± 0.30 | K | NIST Webbook |
| tb | 390.78 ± 0.15 | K | NIST Webbook |
| tb | 390.65 ± 0.50 | K | NIST Webbook |
| tb | 390.78 ± 0.20 | K | NIST Webbook |
| tb | 390.80 ± 0.20 | K | NIST Webbook |
| tb | 390.86 ± 0.20 | K | NIST Webbook |
| tb | 390.70 ± 2.00 | K | NIST Webbook |
| tb | 390.90 | K | NIST Webbook |
| tb | 390.77 ± 0.20 | K | NIST Webbook |
| tc | 561.70 | K | KDB |
| tc | 561.67 ± 0.40 | K | NIST Webbook |
| tc | 561.70 ± 0.50 | K | NIST Webbook |
| tc | 561.70 | K | NIST Webbook |
| tf | 152.17 ± 0.05 | K | NIST Webbook |
| tf | 152.16 ± 0.01 | K | NIST Webbook |
| tf | 152.17 ± 0.06 | K | NIST Webbook |
| tf | 152.06 ± 0.20 | K | NIST Webbook |
| tf | 152.19 ± 0.03 | K | NIST Webbook |
| tf | 151.98 ± 0.30 | K | NIST Webbook |
| tf | 148.85 ± 2.00 | K | NIST Webbook |
| tf | 152.07 ± 0.15 | K | NIST Webbook |
| tf | 148.85 ± 0.30 | K | NIST Webbook |

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|---|---|---|---|
| tf | 152.06 ± 0.30 | K | NIST Webbook |
| tf | 152.00 | K | KDB |
| vc | 0.476 | m3/kmol | NIST Webbook |
| vc | 0.476 | m3/kmol | KDB |
| zc | 0.2588810 | | KDB |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 305.46 | J/mol×K | 549.20 | Joback Method |
| cpg | 245.53 | J/mol×K | 409.87 | Joback Method |
| cpg | 258.44 | J/mol×K | 437.73 | Joback Method |
| cpg | 270.88 | J/mol×K | 465.60 | Joback Method |
| cpg | 282.86 | J/mol×K | 493.46 | Joback Method |
| cpg | 294.38 | J/mol×K | 521.33 | Joback Method |
| cpg | 232.14 | J/mol×K | 382.00 | Joback Method |
| cpl | 251.08 | J/mol×K | 298.15 | NIST Webbook |
| dvisc | 0.0003209 | Pa×s | 345.82 | Joback Method |
| dvisc | 0.0004656 | Pa×s | 309.64 | Joback Method |
| dvisc | 0.0007454 | Pa×s | 273.46 | Joback Method |
| dvisc | 0.0013776 | Pa×s | 237.28 | Joback Method |
| dvisc | 0.0031758 | Pa×s | 201.10 | Joback Method |
| dvisc | 0.0002373 | Pa×s | 382.00 | Joback Method |
| dvisc | 0.0105616 | Pa×s | 164.92 | Joback Method |
| hfust | 10.84 | kJ/mol | 152.20 | NIST Webbook |
| hfust | 10.84 | kJ/mol | 152.20 | NIST Webbook |
| hvapt | 42.30 | kJ/mol | 322.00 | NIST Webbook |
| hvapt | 33.35 | kJ/mol | 390.90 | NIST Webbook |
| hvapt | 33.89 | kJ/mol | 390.90 | KDB |
| hvapt | 38.70 ± 0.10 | kJ/mol | 313.00 | NIST Webbook |
| hvapt | 38.20 | kJ/mol | 352.00 | NIST Webbook |
| hvapt | 36.10 ± 0.10 | kJ/mol | 353.00 | NIST Webbook |
| hvapt | 37.40 ± 0.10 | kJ/mol | 333.00 | NIST Webbook |
| rfi | 1.39553 | | 298.15 | KDB |
| rhol | 705.00 | kg/m3 | 293.00 | KDB |
| srf | 0.02 | N/m | 298.20 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.43890e+01 |
| Coeff. B | -3.39289e+03 |
| Coeff. C | -4.36080e+01 |
| Temperature range (K), min. | 284.21 |
| Temperature range (K), max. | 417.38 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 8.98808e+01 |
| Coeff. B | -7.72965e+03 |
| Coeff. C | -1.11685e+01 |
| Coeff. D | 7.67739e-06 |
| Temperature range (K), min. | 152.20 |
| Temperature range (K), max. | 561.74 |

# Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol49.mol

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C589537&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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=49

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

**af:** Acentric Factor

| | |
|---|---|
| **ap:** | Aniline Point |
| **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 |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **rfi:** | Refractive Index |
| **rhoc:** | Critical density |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **srf:** | Surface Tension |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |
| **zc:** | Critical Compressibility |