

# Hexane, 3,3-dimethyl-

|                      |                                              |
|----------------------|----------------------------------------------|
| Other names:         | 3,3-Dimethylhexane                           |
| Inchi:               | InChI=1S/C8H18/c1-5-7-8(3,4)6-2/h5-7H2,1-4H3 |
| InchiKey:            | KUMXLFI BWFCMOJ-UHFFFAOYSA-N                 |
| Formula:             | C8H18                                        |
| SMILES:              | CCCC(C)(C)CC                                 |
| Mol. weight [g/mol]: | 114.23                                       |
| CAS:                 | 563-16-6                                     |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| af            | 0.3200          |        | KDB            |
| ap            | 345.150         | K      | KDB            |
| chl           | -5462.97 ± 0.96 | kJ/mol | NIST Webbook   |
| gf            | 13.27           | kJ/mol | KDB            |
| hcg           | 5462.97         | kJ/mol | KDB            |
| hcn           | 5066.824        | kJ/mol | KDB            |
| hf            | -220.30         | kJ/mol | KDB            |
| hf            | -220.10 ± 1.10  | kJ/mol | NIST Webbook   |
| hfl           | -257.70 ± 1.10  | kJ/mol | NIST Webbook   |
| hfus          | 9.06            | kJ/mol | Joback Method  |
| hvap          | 37.50 ± 0.10    | kJ/mol | NIST Webbook   |
| hvap          | 37.53           | kJ/mol | NIST Webbook   |
| hvap          | 37.60           | kJ/mol | NIST Webbook   |
| log10ws       | -2.93           |        | Crippen Method |
| logp          | 3.223           |        | Crippen Method |
| mcvol         | 123.580         | ml/mol | McGowan Method |
| pc            | 2653.40 ± 40.53 | kPa    | NIST Webbook   |
| pc            | 2650.00 ± 40.00 | kPa    | NIST Webbook   |
| pc            | 2650.00         | kPa    | KDB            |
| rhoc          | 258.16 ± 4.57   | kg/m3  | NIST Webbook   |
| rhoc          | 258.16 ± 4.57   | kg/m3  | NIST Webbook   |
| rinpol        | 743.00          |        | NIST Webbook   |
| rinpol        | 741.00          |        | NIST Webbook   |
| rinpol        | 743.00          |        | NIST Webbook   |
| rinpol        | 743.10          |        | NIST Webbook   |
| rinpol        | 745.20          |        | NIST Webbook   |
| rinpol        | 743.00          |        | NIST Webbook   |

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|--------|--------|--------------|
| rinpol | 744.00 | NIST Webbook |
| rinpol | 745.00 | NIST Webbook |
| rinpol | 740.40 | NIST Webbook |
| rinpol | 741.20 | NIST Webbook |
| rinpol | 741.80 | NIST Webbook |
| rinpol | 742.90 | NIST Webbook |
| rinpol | 738.00 | NIST Webbook |
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| rinpol | 740.00 | NIST Webbook |
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| rinpol | 743.30 | NIST Webbook |
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| rinpol | 746.00 | NIST Webbook |
| rinpol | 747.40 | NIST Webbook |
| rinpol | 748.70 | NIST Webbook |
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| rinpol | 746.00 | NIST Webbook |
| rinpol | 747.60 | NIST Webbook |
| rinpol | 749.57 | NIST Webbook |
| rinpol | 751.28 | NIST Webbook |
| rinpol | 744.29 | NIST Webbook |
| rinpol | 745.86 | NIST Webbook |
| rinpol | 742.00 | NIST Webbook |
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| rinpol | 746.00 | NIST Webbook |
| rinpol | 742.00 | NIST Webbook |
| rinpol | 744.00 | NIST Webbook |
| rinpol | 746.00 | NIST Webbook |
| rinpol | 735.00 | NIST Webbook |
| rinpol | 742.00 | NIST Webbook |
| rinpol | 738.30 | NIST Webbook |
| rinpol | 741.60 | NIST Webbook |
| rinpol | 735.27 | NIST Webbook |
| rinpol | 735.71 | NIST Webbook |
| rinpol | 739.20 | NIST Webbook |
| rinpol | 744.00 | NIST Webbook |
| rinpol | 736.45 | NIST Webbook |
| rinpol | 743.00 | NIST Webbook |
| rinpol | 735.00 | NIST Webbook |
| rinpol | 739.00 | NIST Webbook |
| rinpol | 740.00 | NIST Webbook |
| rinpol | 744.00 | NIST Webbook |
| rinpol | 741.00 | NIST Webbook |
| rinpol | 743.00 | NIST Webbook |
| rinpol | 750.00 | NIST Webbook |
| rinpol | 746.00 | NIST Webbook |
| rinpol | 736.00 | NIST Webbook |
| rinpol | 742.00 | NIST Webbook |
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| rinpol | 748.00 | NIST Webbook |
| rinpol | 744.00 | NIST Webbook |
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| rinpol | 739.00 | NIST Webbook |
| rinpol | 738.00 | NIST Webbook |
| rinpol | 737.00 | NIST Webbook |
| rinpol | 740.00 | NIST Webbook |
| rinpol | 741.00 | NIST Webbook |
| rinpol | 748.00 | NIST Webbook |
| rinpol | 737.00 | NIST Webbook |
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|--------|-------------------|---|--------------|
| rinpol | 738.30            |   | NIST Webbook |
| rinpol | 738.60            |   | NIST Webbook |
| rinpol | 743.00            |   | NIST Webbook |
| rinpol | 741.20            |   | NIST Webbook |
| rinpol | 744.00            |   | NIST Webbook |
| rinpol | 742.90            |   | NIST Webbook |
| rinpol | 744.29            |   | NIST Webbook |
| rinpol | 739.00            |   | NIST Webbook |
| rinpol | 743.00            |   | NIST Webbook |
| rinpol | 743.00            |   | NIST Webbook |
| rinpol | 743.00            |   | NIST Webbook |
| rinpol | 742.80            |   | NIST Webbook |
| rinpol | 742.90            |   | NIST Webbook |
| rinpol | 740.00            |   | NIST Webbook |
| rinpol | 747.60            |   | NIST Webbook |
| rinpol | 737.00            |   | NIST Webbook |
| rinpol | 737.00            |   | NIST Webbook |
| rinpol | 741.10            |   | NIST Webbook |
| rinpol | 738.60            |   | NIST Webbook |
| rinpol | 741.00            |   | NIST Webbook |
| rinpol | 736.36            |   | NIST Webbook |
| rinpol | 746.00            |   | NIST Webbook |
| tb     | 385.10            | K | NIST Webbook |
| tb     | $385.35 \pm 0.30$ | K | NIST Webbook |
| tb     | $385.10 \pm 0.15$ | K | NIST Webbook |
| tb     | $393.05 \pm 0.50$ | K | NIST Webbook |
| tb     | $385.11 \pm 0.01$ | K | NIST Webbook |
| tb     | $385.35 \pm 0.50$ | K | NIST Webbook |
| tb     | $385.12 \pm 0.10$ | K | NIST Webbook |
| tb     | $385.05 \pm 0.30$ | K | NIST Webbook |
| tb     | $385.15 \pm 0.50$ | K | NIST Webbook |
| tb     | $385.20 \pm 0.50$ | K | NIST Webbook |
| tb     | $384.10 \pm 0.60$ | K | NIST Webbook |
| tb     | $385.12 \pm 0.20$ | K | NIST Webbook |
| tb     | $385.13 \pm 0.10$ | K | NIST Webbook |
| tb     | $384.65 \pm 0.60$ | K | NIST Webbook |
| tb     | $384.65 \pm 1.50$ | K | NIST Webbook |
| tb     | 385.12            | K | KDB          |
| tb     | $385.05 \pm 0.30$ | K | NIST Webbook |
| tb     | 385.20            | K | NIST Webbook |
| tb     | $385.00 \pm 0.30$ | K | NIST Webbook |
| tc     | $562.00 \pm 0.50$ | K | NIST Webbook |
| tc     | 562.00            | K | KDB          |
| tc     | $561.95 \pm 0.40$ | K | NIST Webbook |

|    |               |         |              |
|----|---------------|---------|--------------|
| tf | 147.02 ± 0.01 | K       | NIST Webbook |
| tf | 146.97 ± 0.10 | K       | NIST Webbook |
| tf | 146.98 ± 0.30 | K       | NIST Webbook |
| tf | 147.04 ± 0.02 | K       | NIST Webbook |
| tf | 147.04 ± 0.03 | K       | NIST Webbook |
| tf | 147.00        | K       | KDB          |
| tf | 146.99 ± 0.06 | K       | NIST Webbook |
| tf | 147.04 ± 0.02 | K       | NIST Webbook |
| vc | 0.443         | m3/kmol | NIST Webbook |
| vc | 0.443         | m3/kmol | KDB          |
| zc | 0.2512330     |         | KDB          |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 311.30    | J/mol×K | 553.39          | Joback Method |
| cpg           | 261.70    | J/mol×K | 437.27          | Joback Method |
| cpg           | 275.00    | J/mol×K | 466.30          | Joback Method |
| cpg           | 287.68    | J/mol×K | 495.33          | Joback Method |
| cpg           | 299.78    | J/mol×K | 524.36          | Joback Method |
| cpg           | 233.16    | J/mol×K | 379.21          | Joback Method |
| cpg           | 247.76    | J/mol×K | 408.24          | Joback Method |
| cpl           | 246.60    | J/mol×K | 298.15          | NIST Webbook  |
| dvisc         | 0.0002773 | Pa×s    | 379.21          | Joback Method |
| dvisc         | 0.0005696 | Pa×s    | 313.59          | Joback Method |
| dvisc         | 0.0009261 | Pa×s    | 280.77          | Joback Method |
| dvisc         | 0.0017124 | Pa×s    | 247.96          | Joback Method |
| dvisc         | 0.0038192 | Pa×s    | 215.15          | Joback Method |
| dvisc         | 0.0003841 | Pa×s    | 346.40          | Joback Method |
| dvisc         | 0.0113690 | Pa×s    | 182.34          | Joback Method |
| hvapt         | 41.20     | kJ/mol  | 316.00          | NIST Webbook  |
| hvapt         | 36.60     | kJ/mol  | 347.00          | NIST Webbook  |
| hvapt         | 32.31     | kJ/mol  | 385.10          | NIST Webbook  |
| hvapt         | 32.47     | kJ/mol  | 385.10          | KDB           |
| rfi           | 1.39782   |         | 298.15          | KDB           |
| rhoI          | 710.00    | 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                    | 1.42437e+01                   |
| Coeff. B                    | -3.31817e+03                  |
| Coeff. C                    | -4.03870e+01                  |
| Temperature range (K), min. | 278.15                        |
| Temperature range (K), max. | 411.87                        |

| Information                 | Value                                                  |
|-----------------------------|--------------------------------------------------------|
| Property code               | pvap                                                   |
| Equation                    | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A                    | 8.59858e+01                                            |
| Coeff. B                    | -7.31793e+03                                           |
| Coeff. C                    | -1.06713e+01                                           |
| Coeff. D                    | 7.86020e-06                                            |
| Temperature range (K), min. | 147.05                                                 |
| Temperature range (K), max. | 562.00                                                 |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Joback Method:                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| KDB:                                 | <a href="https://www.thermo.com/files/research/kdb/mol/mol55.mol">https://www.thermo.com/files/research/kdb/mol/mol55.mol</a>                                                           |
| McGowan Method:                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C563166&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C563166&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> |
| KDB Vapor Pressure Data:             | <a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=55">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=55</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.chemed.com/doc/models/crippen_log10ws">https://www.chemed.com/doc/models/crippen_log10ws</a>                                                                       |

## Legend

af: Acentric Factor

|                 |                                                           |
|-----------------|-----------------------------------------------------------|
| <b>ap:</b>      | Aniline Point                                             |
| <b>chl:</b>     | Standard liquid enthalpy of combustion                    |
| <b>cpg:</b>     | Ideal gas heat capacity                                   |
| <b>cpl:</b>     | Liquid phase 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>hfl:</b>     | Liquid phase 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>log10ws:</b> | Log10 of Water solubility in mol/l                        |
| <b>logp:</b>    | Octanol/Water partition coefficient                       |
| <b>mccvol:</b>  | McGowan's characteristic volume                           |
| <b>pc:</b>      | Critical Pressure                                         |
| <b>pvap:</b>    | Vapor pressure                                            |
| <b>rfi:</b>     | Refractive Index                                          |
| <b>rhoc:</b>    | Critical density                                          |
| <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                             |
| <b>vc:</b>      | Critical Volume                                           |
| <b>zc:</b>      | Critical Compressibility                                  |

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