

# 1-Tetradecene

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | N-TETRADEC-1-ENE<br>Neodene 14<br>Tetradec-1-ene<br>Tetradecene-1<br>«alpha»-Tetradecene<br>Â«alphaÂ»-Tetradecene |
| <b>Inchi:</b>               | InChI=1S/C14H28/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3H,1,4-14H2,2H3  |
| <b>InchiKey:</b>            | HFDVRLIODXPAHB-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C14H28  |
| <b>SMILES:</b>              | C=CCCCCCCCCCCCC   |
| <b>Mol. weight [g/mol]:</b> | 196.37  |
| <b>CAS:</b>                 | 1120-36-1   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| af            | 0.6440  |        | KDB            |
| gf            | 154.90  | kJ/mol | KDB            |
| hf            | -206.70 | kJ/mol | KDB            |
| hfus          | 30.74   | kJ/mol | Joback Method  |
| hvap          | 70.20   | kJ/mol | NIST Webbook   |
| log10ws       | -5.54   |        | Crippen Method |
| logp          | 5.483   |        | Crippen Method |
| mcvol         | 203.820 | ml/mol | McGowan Method |
| pc            | 1560.00 | kPa    | KDB            |
| rinpol        | 1389.46 |        | NIST Webbook   |
| rinpol        | 1387.00 |        | NIST Webbook   |
| rinpol        | 1395.00 |        | NIST Webbook   |
| rinpol        | 1396.00 |        | NIST Webbook   |
| rinpol        | 1392.00 |        | NIST Webbook   |
| rinpol        | 1394.00 |        | NIST Webbook   |
| rinpol        | 1397.00 |        | NIST Webbook   |
| rinpol        | 1389.35 |        | NIST Webbook   |
| rinpol        | 1391.70 |        | NIST Webbook   |
| rinpol        | 1391.20 |        | NIST Webbook   |
| rinpol        | 1389.00 |        | NIST Webbook   |
| rinpol        | 1393.00 |        | NIST Webbook   |
| rinpol        | 1390.00 |        | NIST Webbook   |

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| rinpol | 238.00  | NIST Webbook |
| rinpol | 1389.00 | NIST Webbook |
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| rinpol | 1389.00 | NIST Webbook |
| rinpol | 1392.68 | NIST Webbook |
| rinpol | 1392.49 | NIST Webbook |
| rinpol | 1392.25 | NIST Webbook |
| rinpol | 1383.00 | NIST Webbook |
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| rinpol | 1388.00 | NIST Webbook |
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| ripol | 1434.70 | NIST Webbook |
| ripol | 1431.40 | NIST Webbook |
| ripol | 1441.90 | NIST Webbook |
| ripol | 1440.90 | NIST Webbook |
| ripol | 1443.60 | NIST Webbook |
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| ripol | 1428.70 | NIST Webbook |
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| ripol | 1442.10 | NIST Webbook |
| ripol | 1431.90 | NIST Webbook |
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| ripol | 1454.00       |                      | NIST Webbook |
| ripol | 1442.00       |                      | NIST Webbook |
| tb    | 524.20        | K                    | NIST Webbook |
| tb    | 524.30        | K                    | KDB          |
| tb    | 524.00        | K                    | NIST Webbook |
| tc    | 689.00        | K                    | KDB          |
| tf    | 260.23 ± 0.06 | K                    | NIST Webbook |
| tf    | 260.23 ± 0.06 | K                    | NIST Webbook |
| tf    | 260.23 ± 0.05 | K                    | NIST Webbook |
| tf    | 260.30 ± 0.03 | K                    | NIST Webbook |
| tf    | 260.00        | K                    | KDB          |
| tf    | 260.30 ± 0.04 | K                    | NIST Webbook |
| vc    | 0.800         | m <sup>3</sup> /kmol | KDB          |
| zc    | 0.2179870     |                      | KDB          |

## Temperature Dependent Properties

| Property code | Value     | Unit              | Temperature [K] | Source        |
|---------------|-----------|-------------------|-----------------|---------------|
| cpg           | 486.57    | J/mol×K           | 516.40          | Joback Method |
| cpg           | 504.23    | J/mol×K           | 543.43          | Joback Method |
| cpg           | 521.19    | J/mol×K           | 570.47          | Joback Method |
| cpg           | 537.47    | J/mol×K           | 597.50          | Joback Method |
| cpg           | 553.09    | J/mol×K           | 624.54          | Joback Method |
| cpg           | 568.07    | J/mol×K           | 651.57          | Joback Method |
| cpg           | 582.43    | J/mol×K           | 678.61          | Joback Method |
| dvisc         | 0.0009515 | Paxs              | 335.99          | Joback Method |
| dvisc         | 0.0019579 | Paxs              | 290.88          | Joback Method |
| dvisc         | 0.0052502 | Paxs              | 245.78          | Joback Method |
| dvisc         | 0.0005486 | Paxs              | 381.09          | Joback Method |
| dvisc         | 0.0003554 | Paxs              | 426.19          | Joback Method |
| dvisc         | 0.0002501 | Paxs              | 471.30          | Joback Method |
| dvisc         | 0.0001872 | Paxs              | 516.40          | Joback Method |
| hvapt         | 46.90     | kJ/mol            | 524.30          | KDB           |
| hvapt         | 56.50     | kJ/mol            | 478.50          | NIST Webbook  |
| rhoI          | 786.00    | kg/m <sup>3</sup> | 273.00          | KDB           |
| srf           | 0.03      | N/m               | 298.20          | KDB           |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 398.20 | K    | 2.00           | NIST Webbook |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.47321e+01                   |
| Coeff. B                    | -4.43698e+03                  |
| Coeff. C                    | -8.54930e+01                  |
| Temperature range (K), min. | 392.67                        |
| Temperature range (K), max. | 556.48                        |

| Information                 | Value  |
|-----------------------------|--|
| Property code               | pvap   |
| Equation                    | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A                    | 1.63674e+02  |
| Coeff. B                    | -1.45730e+04   |
| Coeff. C                    | -2.13939e+01   |
| Coeff. D                    | 9.84515e-06  |
| Temperature range (K), min. | 260.30   |
| Temperature range (K), max. | 692.00   |

## Sources

Infinite dilution activity coefficients, specific retention volumes and vapor pressure data for the dynamics of hydrocarbons in C<sub>7</sub>H<sub>15</sub> branched alkane solvent.

KDB:

Crippen Method:

The Yaws Handbook of Vapor Pressure:  
NIST Webbook:

<https://www.doi.org/10.1016/j.fluid.2006.07.015>

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=349>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=349>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120361&Units=SI>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

|                 |   |
|-----------------|---|
| <b>af:</b>      | Acentric Factor                                 |
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | 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>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>pvap:</b>    | Vapor pressure                                  |
| <b>rho:</b>     | Liquid Density                                  |
| <b>rinp:</b>    | Non-polar retention indices                     |
| <b>rip:</b>     | Polar retention indices                         |
| <b>srf:</b>     | Surface Tension                                 |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <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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