

# 3-Undecyne

**Other names:** 3-C<sub>11</sub>H<sub>20</sub>  
**Inchi:** InChI=1S/C<sub>11</sub>H<sub>20</sub>/c1-3-5-7-9-11-10-8-6-4-2/h3-5,7,9-11H<sub>2</sub>,1-2H<sub>3</sub>  
**InchiKey:** DPWGJNPCPLQVKQ-UHFFFAOYSA-N  
**Formula:** C<sub>11</sub>H<sub>20</sub>  
**SMILES:** CCC#CCCCCCCC  
**Mol. weight [g/mol]:** 152.28  
**CAS:** 60212-30-8

## Physical Properties

| Property code | Value       | Unit   | Source         |
|---------------|-------------|--------|----------------|
| gf            | 244.54      | kJ/mol | Joback Method  |
| hf            | 1.93        | kJ/mol | Joback Method  |
| hfus          | 27.37       | kJ/mol | Joback Method  |
| hvap          | 42.23       | kJ/mol | Joback Method  |
| ie            | 9.17 ± 0.02 | eV     | NIST Webbook   |
| log10ws       | -4.22       |        | Crippen Method |
| logp          | 3.760       |        | Crippen Method |
| mcvol         | 157.250     | ml/mol | McGowan Method |
| pc            | 2237.64     | kPa    | Joback Method  |
| rinpol        | 1112.00     |        | NIST Webbook   |
| rinpol        | 1119.00     |        | NIST Webbook   |
| rinpol        | 1114.00     |        | NIST Webbook   |
| rinpol        | 1116.00     |        | NIST Webbook   |
| rinpol        | 1117.00     |        | NIST Webbook   |
| rinpol        | 1119.00     |        | NIST Webbook   |
| rinpol        | 1119.00     |        | NIST Webbook   |
| rinpol        | 1111.00     |        | NIST Webbook   |
| rinpol        | 1112.00     |        | NIST Webbook   |
| rinpol        | 1114.00     |        | NIST Webbook   |
| rinpol        | 1138.00     |        | NIST Webbook   |
| ripol         | 1306.00     |        | NIST Webbook   |
| ripol         | 1301.30     |        | NIST Webbook   |
| ripol         | 1305.00     |        | NIST Webbook   |
| ripol         | 1306.00     |        | NIST Webbook   |
| ripol         | 1301.30     |        | NIST Webbook   |
| ripol         | 1285.80     |        | NIST Webbook   |
| ripol         | 1300.00     |        | NIST Webbook   |

|       |         |                      |               |
|-------|---------|----------------------|---------------|
| ripol | 1283.80 |                      | NIST Webbook  |
| ripol | 1281.10 |                      | NIST Webbook  |
| ripol | 1306.00 |                      | NIST Webbook  |
| ripol | 1306.00 |                      | NIST Webbook  |
| ripol | 1305.00 |                      | NIST Webbook  |
| ripol | 1306.00 |                      | NIST Webbook  |
| ripol | 1305.00 |                      | NIST Webbook  |
| tb    | 460.08  | K                    | Joback Method |
| tc    | 642.86  | K                    | Joback Method |
| tf    | 319.83  | K                    | Joback Method |
| vc    | 0.614   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 331.56 | J/mol×K | 460.08          | Joback Method |
| cpg           | 347.02 | J/mol×K | 490.54          | Joback Method |
| cpg           | 361.85 | J/mol×K | 521.01          | Joback Method |
| cpg           | 376.06 | J/mol×K | 551.47          | Joback Method |
| cpg           | 389.69 | J/mol×K | 581.93          | Joback Method |
| cpg           | 402.74 | J/mol×K | 612.39          | Joback Method |
| cpg           | 415.23 | J/mol×K | 642.86          | Joback Method |

## Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 353.00 ± 1.00 | K    | 1.30           | NIST Webbook |

## Correlations

| Information   | Value                         |
|---------------|-------------------------------|
| Property code | pvap                          |
| Equation      | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A      | 1.54172e+01                   |
| Coeff. B      | -4.32455e+03                  |

|                             |              |
|-----------------------------|--------------|
| Coeff. C                    | -7.26860e+01 |
| Temperature range (K), min. | 358.52       |
| Temperature range (K), max. | 500.62       |

## Sources

|   |   |
|---|---|
| <b>The Yaws Handbook of Vapor Pressure:</b> | <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> |
| <b>Crippen Method:</b>                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>   |
| <b>Crippen Method:</b>                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>   |
| <b>Joback Method:</b>                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>   |
| <b>McGowan Method:</b>                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>   |
| <b>NIST Webbook:</b>                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C60212308&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C60212308&amp;Units=SI</a>   |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>ie:</b>      | Ionization energy                               |
| <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>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <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                                 |

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