

# Nonadecane, 5-methyl

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 5-methylnonadecane<br>Hexadecane, 2-butyl   |
| <b>Inchi:</b>               | InChI=1S/C20H42/c1-4-6-8-9-10-11-12-13-14-15-16-17-19-20(3)18-7-5-2/h20H,4-19H2,1 |
| <b>InchiKey:</b>            | ZFWCHSBHHWYGCK-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C20H42  |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCC(C)CCCC  |
| <b>Mol. weight [g/mol]:</b> | 282.55  |
| <b>CAS:</b>                 | 57160-72-2  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 115.08  | kJ/mol  | Joback Method  |
| hf            | -461.41 | kJ/mol  | Joback Method  |
| hfus          | 44.03   | kJ/mol  | Joback Method  |
| hvap          | 59.73   | kJ/mol  | Joback Method  |
| log10ws       | -7.95   |         | Crippen Method |
| logp          | 7.904   |         | Crippen Method |
| mcvol         | 292.660 | ml/mol  | McGowan Method |
| pc            | 1020.73 | kPa     | Joback Method  |
| rinpol        | 1953.40 |         | NIST Webbook   |
| rinpol        | 1952.00 |         | NIST Webbook   |
| rinpol        | 1946.60 |         | NIST Webbook   |
| rinpol        | 1953.00 |         | NIST Webbook   |
| rinpol        | 1951.60 |         | NIST Webbook   |
| rinpol        | 1953.00 |         | NIST Webbook   |
| rinpol        | 1948.00 |         | NIST Webbook   |
| ripol         | 1948.70 |         | NIST Webbook   |
| tb            | 656.56  | K       | Joback Method  |
| tc            | 818.58  | K       | Joback Method  |
| tf            | 300.16  | K       | Joback Method  |
| vc            | 1.149   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 840.82    | J/mol×K | 656.56          | Joback Method |
| cpg           | 862.00    | J/mol×K | 683.56          | Joback Method |
| cpg           | 882.29    | J/mol×K | 710.57          | Joback Method |
| cpg           | 901.73    | J/mol×K | 737.57          | Joback Method |
| cpg           | 920.35    | J/mol×K | 764.58          | Joback Method |
| cpg           | 938.17    | J/mol×K | 791.58          | Joback Method |
| cpg           | 955.21    | J/mol×K | 818.58          | Joback Method |
| dvisc         | 0.0051032 | Paxs    | 300.16          | Joback Method |
| dvisc         | 0.0014944 | Paxs    | 359.56          | Joback Method |
| dvisc         | 0.0006199 | Paxs    | 418.96          | Joback Method |
| dvisc         | 0.0003200 | Paxs    | 478.36          | Joback Method |
| dvisc         | 0.0001911 | Paxs    | 537.76          | Joback Method |
| dvisc         | 0.0001265 | Paxs    | 597.16          | Joback Method |
| dvisc         | 0.0000902 | Paxs    | 656.56          | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.82211e+01                   |
| Coeff. B                    | -8.27437e+03                  |
| Coeff. C                    | -8.86000e-01                  |
| Temperature range (K), min. | 462.28                        |
| Temperature range (K), max. | 641.83                        |

## Sources

**McGowan Method:**

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

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R31622&Units=SI>

**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/ci9903071>

**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>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>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>rinpolar:</b> | Non-polar retention indices                     |
| <b>ripolar:</b>  | Polar retention indices                         |
| <b>tb:</b>       | Normal Boiling Point Temperature                |
| <b>tc:</b>       | Critical Temperature                            |
| <b>tf:</b>       | Normal melting (fusion) point                   |
| <b>vc:</b>       | Critical Volume                                 |

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