# Nonadecylbenzene

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|---|---|
| **Other names:** | 1-phenylnonadecane<br>Nonadecane, 1-phenyl-<br>benzene, nondecyl-<br>n-Nonadecylbenzene |
| **Inchi:** | InChI=1S/C25H44/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-22-25-23-20-18-21-24 |
| **InchiKey:** | SHWJJBRTHGGZBE-UHFFFAOYSA-N |
| **Formula:** | C25H44 |
| **SMILES:** | CCCCCCCCCCCCCCCCCCCCc1ccccc1 |
| **Mol. weight [g/mol]:** | 344.63 |
| **CAS:** | 29136-19-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.9895 | | Cheméo Relay (1.0) |
| gf | 272.03 | kJ/mol | Joback Method |
| hf | -312.62 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 54.55 | kJ/mol | Joback Method |
| hvap | 122.21 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.23 | eV | Cheméo Relay (1.0) |
| log10ws | -9.12 | | Cheméo Relay (1.0) |
| logp | 8.881 | | Crippen Method |
| mcvol | 339.350 | ml/mol | McGowan Method |
| pc | 925.55 | kPa | Joback Method |
| tb | 639.13 | K | Cheméo Relay (1.0) |
| tc | 823.05 | K | Cheméo Relay (1.0) |
| tf | 298.16 ± 0.40 | K | NIST Webbook |
| tf | 298.10 ± 0.03 | K | NIST Webbook |
| tf | 302.70 ± 0.04 | K | NIST Webbook |
| vc | 1.339 | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1069.33 | J/mol×K | 798.08 | Joback Method |

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|---|---|---|---|---|
| cpg | 1182.19 | J/mol×K | 983.47 | Joback Method |
| cpg | 1165.84 | J/mol×K | 952.57 | Joback Method |
| cpg | 1148.57 | J/mol×K | 921.68 | Joback Method |
| cpg | 1130.35 | J/mol×K | 890.78 | Joback Method |
| cpg | 1111.10 | J/mol×K | 859.88 | Joback Method |
| cpg | 1090.78 | J/mol×K | 828.98 | Joback Method |
| dvisc | 0.0001589 | Pa×s | 598.00 | Joback Method |
| dvisc | 0.0000513 | Pa×s | 798.08 | Joback Method |
| dvisc | 0.0000698 | Pa×s | 731.39 | Joback Method |
| dvisc | 0.0001011 | Pa×s | 664.70 | Joback Method |
| dvisc | 0.0015356 | Pa×s | 397.93 | Joback Method |
| dvisc | 0.0002800 | Pa×s | 531.31 | Joback Method |
| dvisc | 0.0005803 | Pa×s | 464.62 | Joback Method |
| hvapt | 103.60 | kJ/mol | 558.50 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tfp | 302.60 | K | 100.00 | Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes |
| tfp | 307.20 | K | 20000.00 | Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes |
| tfp | 311.60 | K | 40200.00 | Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes |
| tfp | 319.70 | K | 80200.00 | Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes |
| tfp | 322.90 | K | 99600.00 | Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.36049e+01 |
| Coeff. B | -4.57796e+03 |
| Coeff. C | -1.78408e+02 |
| Temperature range (K), min. | 522.17 |
| Temperature range (K), max. | 730.40 |

# Sources

| | |
|---|---|
| **Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes:** | https://www.doi.org/10.1021/je700529y |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C29136194&Units=SI |
| **Cheméo Relay (1.0, beta):** | |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Cheméo Relay (1.0):** | |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |

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|---|---|
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tfp:** | Melting point |
| **vc:** | Critical Volume |