# 1-Octadecene

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|---|---|
| **Other names:** | Neodene 18 |
| | Octadec-1-ene |
| | Octadeca-1-ene |
| | Octadecene-1 |
| | Octadecylene, «alpha»- |
| | Octadecylene, Â«alphaÂ»- |
| | «alpha»-Octadecene |
| | Â«alphaÂ»-Octadecene |
| **Inchi:** | InChI=1S/C18H36/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h3H,1,4-18H2,2H3 |
| **InchiKey:** | CCCMONHAUSKTEQ-UHFFFAOYSA-N |
| **Formula:** | C18H36 |
| **SMILES:** | C=CCCCCCCCCCCCCCCCC |
| **Mol. weight [g/mol]:** | 252.48 |
| **CAS:** | 112-88-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.8070 | | KDB |
| gf | 188.40 | kJ/mol | KDB |
| hf | -289.20 | kJ/mol | KDB |
| hfus | 41.10 | kJ/mol | Joback Method |
| hvap | 90.00 | kJ/mol | NIST Webbook |
| log10ws | -7.21 | | Crippen Method |
| logp | 7.044 | | Crippen Method |
| mcvol | 260.180 | ml/mol | McGowan Method |
| pc | 1130.00 | kPa | KDB |
| rinpol | 1786.80 | | NIST Webbook |
| rinpol | 1787.80 | | NIST Webbook |
| rinpol | 1790.00 | | NIST Webbook |
| rinpol | 1795.00 | | NIST Webbook |
| rinpol | 1793.00 | | NIST Webbook |
| rinpol | 1794.00 | | NIST Webbook |
| rinpol | 1786.00 | | NIST Webbook |
| rinpol | 1793.00 | | NIST Webbook |
| rinpol | 1792.10 | | NIST Webbook |
| rinpol | 1792.10 | | NIST Webbook |
| rinpol | 1792.60 | | NIST Webbook |

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|---|---|---|
| rinpol | 1792.10 | NIST Webbook |
| rinpol | 1793.50 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| rinpol | 1788.00 | NIST Webbook |
| rinpol | 1792.60 | NIST Webbook |
| rinpol | 1792.10 | NIST Webbook |
| rinpol | 1793.50 | NIST Webbook |
| rinpol | 1792.10 | NIST Webbook |
| rinpol | 1792.10 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| rinpol | 1788.00 | NIST Webbook |
| rinpol | 1794.00 | NIST Webbook |
| rinpol | 1791.00 | NIST Webbook |
| rinpol | 1792.00 | NIST Webbook |
| rinpol | 1793.10 | NIST Webbook |
| rinpol | 1794.00 | NIST Webbook |
| rinpol | 1791.00 | NIST Webbook |
| rinpol | 1791.00 | NIST Webbook |
| rinpol | 1788.00 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| rinpol | 1792.00 | NIST Webbook |
| rinpol | 1788.00 | NIST Webbook |
| rinpol | 1790.00 | NIST Webbook |
| rinpol | 1792.00 | NIST Webbook |
| rinpol | 1800.00 | NIST Webbook |
| rinpol | 1792.00 | NIST Webbook |
| rinpol | 1788.00 | NIST Webbook |
| rinpol | 1792.00 | NIST Webbook |
| rinpol | 1805.00 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| rinpol | 1789.00 | NIST Webbook |
| rinpol | 1790.00 | NIST Webbook |
| rinpol | 1779.00 | NIST Webbook |
| rinpol | 1795.00 | NIST Webbook |
| rinpol | 1799.00 | NIST Webbook |
| rinpol | 1795.00 | NIST Webbook |
| rinpol | 1792.10 | NIST Webbook |
| rinpol | 1793.50 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| rinpol | 1793.00 | NIST Webbook |
| ripol | 1856.00 | NIST Webbook |

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|---|---|---|---|
| ripol | 1824.00 | | NIST Webbook |
| ripol | 1848.00 | | NIST Webbook |
| ripol | 1823.00 | | NIST Webbook |
| ripol | 1862.00 | | NIST Webbook |
| ripol | 1824.00 | | NIST Webbook |
| ripol | 1862.00 | | NIST Webbook |
| tb | 588.00 | K | KDB |
| tc | 739.00 | K | KDB |
| tf | 290.80 | K | KDB |
| tf | 291.00 ± 3.00 | K | NIST Webbook |
| vc | 1.024 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 791.64 | J/mol×K | 741.79 | Joback Method |
| cpg | 807.53 | J/mol×K | 768.56 | Joback Method |
| cpg | 701.21 | J/mol×K | 607.92 | Joback Method |
| cpg | 720.85 | J/mol×K | 634.69 | Joback Method |
| cpg | 739.69 | J/mol×K | 661.47 | Joback Method |
| cpg | 757.75 | J/mol×K | 688.24 | Joback Method |
| cpg | 775.06 | J/mol×K | 715.02 | Joback Method |
| dvisc | 0.0001733 | Pa×s | 555.08 | Joback Method |
| dvisc | 0.0001279 | Pa×s | 607.92 | Joback Method |
| dvisc | 0.0041476 | Pa×s | 290.86 | Joback Method |
| dvisc | 0.0014873 | Pa×s | 343.70 | Joback Method |
| dvisc | 0.0007010 | Pa×s | 396.55 | Joback Method |
| dvisc | 0.0003943 | Pa×s | 449.39 | Joback Method |
| dvisc | 0.0002504 | Pa×s | 502.23 | Joback Method |
| hvapt | 76.40 | kJ/mol | 494.00 | NIST Webbook |
| hvapt | 54.27 | kJ/mol | 588.00 | KDB |
| rhol | 789.00 | kg/m3 | 293.00 | KDB |
| srf | 0.03 | N/m | 298.20 | KDB |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 452.00 | K | 2.00 | NIST Webbook |

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|---|---|---|---|---|
| tbrp | 452.20 | K | 2.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.55323e+01 |
| Coeff. B | -5.05557e+03 |
| Coeff. C | -1.15594e+02 |
| Temperature range (K), min. | 447.22 |
| Temperature range (K), max. | 610.23 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 2.79261e+02 |
| Coeff. B | -2.28693e+04 |
| Coeff. C | -3.78359e+01 |
| Coeff. D | 1.59356e-05 |
| Temperature range (K), min. | 290.76 |
| Temperature range (K), max. | 748.00 |

# Sources

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|---|---|
| **KDB:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=353 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=353 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C112889&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **KDB Pure (Korean Thermophysical Properties Databank):** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=353 |

# 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 |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **srf:** | Surface Tension |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |