# Phenanthrene, 1-methyl-

**Other names:** 1-Methylphenanthrene
**Inchi:** InChI=1S/C15H12/c1-11-5-4-8-15-13(11)10-9-12-6-2-3-7-14(12)15/h2-10H,1H3
**InchiKey:** DOWJXOHBNXRUOD-UHFFFAOYSA-N
**Formula:** C15H12
**SMILES:** Cc1cccc2c1ccc1ccccc12
**Mol. weight [g/mol]:** 192.26
**CAS:** 832-69-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 381.87 | kJ/mol | Joback Method |
| hf | 242.80 | kJ/mol | Joback Method |
| hfus | 21.91 | kJ/mol | Joback Method |
| hvap | 84.50 ± 1.40 | kJ/mol | NIST Webbook |
| ie | 7.70 ± 0.03 | eV | NIST Webbook |
| ie | 7.70 ± 0.03 | eV | NIST Webbook |
| log10ws | -5.85 | | Estimated Solubility Method |
| log10ws | -5.85 | | Aqueous Solubility Prediction Method |
| logp | 4.301 | | Crippen Method |
| mcvol | 159.530 | ml/mol | McGowan Method |
| pc | 2868.87 | kPa | Joback Method |
| rinpol | 1929.00 | | NIST Webbook |
| rinpol | 323.79 | | NIST Webbook |
| rinpol | 323.52 | | NIST Webbook |
| rinpol | 323.67 | | NIST Webbook |
| rinpol | 323.92 | | NIST Webbook |
| rinpol | 324.21 | | NIST Webbook |
| rinpol | 323.78 | | NIST Webbook |
| rinpol | 323.70 | | NIST Webbook |
| rinpol | 323.90 | | NIST Webbook |
| rinpol | 324.00 | | NIST Webbook |
| rinpol | 323.52 | | NIST Webbook |
| rinpol | 323.79 | | NIST Webbook |
| rinpol | 323.64 | | NIST Webbook |
| rinpol | 323.90 | | NIST Webbook |
| rinpol | 321.10 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 323.54 | | NIST Webbook |
| rinpol | 323.52 | | NIST Webbook |
| rinpol | 323.54 | | NIST Webbook |
| rinpol | 323.78 | | NIST Webbook |
| rinpol | 320.00 | | NIST Webbook |
| rinpol | 338.91 | | NIST Webbook |
| rinpol | 323.30 | | NIST Webbook |
| rinpol | 323.30 | | NIST Webbook |
| rinpol | 323.90 | | NIST Webbook |
| rinpol | 323.60 | | NIST Webbook |
| rinpol | 322.61 | | NIST Webbook |
| rinpol | 323.60 | | NIST Webbook |
| rinpol | 323.60 | | NIST Webbook |
| rinpol | 324.60 | | NIST Webbook |
| rinpol | 319.96 | | NIST Webbook |
| rinpol | 323.90 | | NIST Webbook |
| rinpol | 323.91 | | NIST Webbook |
| rinpol | 323.80 | | NIST Webbook |
| rinpol | 321.28 | | NIST Webbook |
| rinpol | 323.60 | | NIST Webbook |
| rinpol | 323.90 | | NIST Webbook |
| rinpol | 323.90 | | NIST Webbook |
| rinpol | 323.59 | | NIST Webbook |
| rinpol | 1896.00 | | NIST Webbook |
| rinpol | 1888.00 | | NIST Webbook |
| rinpol | 1890.00 | | NIST Webbook |
| rinpol | 321.43 | | NIST Webbook |
| rinpol | 1883.00 | | NIST Webbook |
| rinpol | 1944.00 | | NIST Webbook |
| rinpol | 1901.20 | | NIST Webbook |
| tb | 617.20 | K | Joback Method |
| tc | 866.35 | K | Joback Method |
| tf | 375.67 | K | Joback Method |
| vc | 0.612 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 381.22 | J/mol×K | 617.20 | Joback Method |
| cpg | 396.50 | J/mol×K | 658.73 | Joback Method |
| cpg | 410.54 | J/mol×K | 700.25 | Joback Method |

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|---|---|---|---|---|
| cpg | 423.46 | J/mol×K | 741.78 | Joback Method |
| cpg | 435.41 | J/mol×K | 783.30 | Joback Method |
| cpg | 446.52 | J/mol×K | 824.83 | Joback Method |
| cpg | 456.90 | J/mol×K | 866.35 | Joback Method |
| dvisc | 0.0013574 | Pa×s | 375.67 | Joback Method |
| dvisc | 0.0010334 | Pa×s | 415.93 | Joback Method |
| dvisc | 0.0008255 | Pa×s | 456.18 | Joback Method |
| dvisc | 0.0006839 | Pa×s | 496.44 | Joback Method |
| dvisc | 0.0005828 | Pa×s | 536.69 | Joback Method |
| dvisc | 0.0005079 | Pa×s | 576.95 | Joback Method |
| dvisc | 0.0004506 | Pa×s | 617.20 | Joback Method |
| hvapt | 76.30 | kJ/mol | 398.00 | NIST Webbook |
| pvap | 2.20 | kPa | 480.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.71 | kPa | 450.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 1.05 | kPa | 460.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 1.54 | kPa | 470.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.46 | kPa | 440.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |

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|---|---|---|---|---|
| pvap | 3.09 | kPa | 490.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 4.26 | kPa | 500.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 5.79 | kPa | 510.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.29 | kPa | 430.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.18 | kPa | 420.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.11 | kPa | 410.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.06 | kPa | 400.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |

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|---|---|---|---|---|
| pvap | 0.04 | kPa | 390.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.02 | kPa | 380.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.01 | kPa | 370.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 5.07e-03 | kPa | 360.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 2.40e-03 | kPa | 350.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 1.08e-03 | kPa | 340.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 4.56e-04 | kPa | 330.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |

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|---|---|---|---|---|
| pvap | 1.80e-04 | kPa | 320.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 6.66e-05 | kPa | 310.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 2.28e-05 | kPa | 300.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 1.85e-05 | kPa | 298.15 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.38885e+01 |
| Coeff. B | -4.73615e+03 |
| Coeff. C | -1.15498e+02 |
| Temperature range (K), min. | 463.72 |
| Temperature range (K), max. | 667.69 |

# Sources

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|---|---|
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C832699&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/ci990307l |
| **Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:** | https://www.doi.org/10.1021/je800300x |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |

# Legend

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