# 9,10-Dimethylanthracene

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| **Other names:** | 9:10-Dimethylanthracene |
| | Anthracene, 9,10-dimethyl- |
| **Inchi:** | InChI=1S/C16H14/c1-11-13-7-3-5-9-15(13)12(2)16-10-6-4-8-14(11)16/h3-10H,1-2H3 |
| **InchiKey:** | JTGMTYWYUZDRBK-UHFFFAOYSA-N |
| **Formula:** | C16H14 |
| **SMILES:** | Cc1c2ccccc2c(C)c2ccccc12 |
| **Mol. weight [g/mol]:** | 206.28 |
| **CAS:** | 781-43-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 380.66 | kJ/mol | Joback Method |
| hf | 210.69 | kJ/mol | Joback Method |
| hfus | 24.11 | kJ/mol | Joback Method |
| hsub | 113.00 ± 1.70 | kJ/mol | NIST Webbook |
| hvap | 94.50 ± 0.20 | kJ/mol | NIST Webbook |
| log10ws | -6.57 | | Estimated Solubility Method |
| log10ws | -6.57 | | Aqueous Solubility Prediction Method |
| logp | 4.610 | | Crippen Method |
| mcvol | 173.620 | ml/mol | McGowan Method |
| pc | 2555.92 | kPa | Joback Method |
| rinpol | 2106.00 | | NIST Webbook |
| rinpol | 2135.50 | | NIST Webbook |
| rinpol | 2152.60 | | NIST Webbook |
| rinpol | 2135.50 | | NIST Webbook |
| rinpol | 2135.10 | | NIST Webbook |
| rinpol | 2156.00 | | NIST Webbook |
| rinpol | 349.10 | | NIST Webbook |
| rinpol | 2152.60 | | NIST Webbook |
| rinpol | 355.21 | | NIST Webbook |
| rinpol | 355.09 | | NIST Webbook |
| rinpol | 355.49 | | NIST Webbook |
| rinpol | 2107.60 | | NIST Webbook |
| rinpol | 351.98 | | NIST Webbook |
| rinpol | 355.49 | | NIST Webbook |
| rinpol | 2135.50 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 2107.60 | | NIST Webbook |
| rinpol | 2156.70 | | NIST Webbook |
| rinpol | 2135.50 | | NIST Webbook |
| rinpol | 355.70 | | NIST Webbook |
| rinpol | 2135.10 | | NIST Webbook |
| rinpol | 355.59 | | NIST Webbook |
| tb | 645.06 | K | Joback Method |
| tc | 889.67 | K | Joback Method |
| tf | 459.50 | K | Thermochemistry of some alkylsubstituted anthracenes |
| vc | 0.667 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 429.69 | J/mol×K | 645.06 | Joback Method |
| cpg | 445.30 | J/mol×K | 685.83 | Joback Method |
| cpg | 459.74 | J/mol×K | 726.60 | Joback Method |
| cpg | 473.15 | J/mol×K | 767.36 | Joback Method |
| cpg | 485.63 | J/mol×K | 808.13 | Joback Method |
| cpg | 497.31 | J/mol×K | 848.90 | Joback Method |
| cpg | 508.31 | J/mol×K | 889.67 | Joback Method |
| dvisc | 0.0009553 | Pa×s | 440.39 | Joback Method |
| dvisc | 0.0012344 | Pa×s | 399.46 | Joback Method |
| dvisc | 0.0007722 | Pa×s | 481.33 | Joback Method |
| dvisc | 0.0006454 | Pa×s | 522.26 | Joback Method |
| dvisc | 0.0005537 | Pa×s | 563.19 | Joback Method |
| dvisc | 0.0004850 | Pa×s | 604.13 | Joback Method |
| dvisc | 0.0004320 | Pa×s | 645.06 | Joback Method |
| hsubt | 109.40 ± 1.70 | kJ/mol | 370.50 | NIST Webbook |
| hsubt | 114.60 | kJ/mol | 377.00 | NIST Webbook |
| hsubt | 103.20 | kJ/mol | 407.50 | NIST Webbook |
| pvap | 3.25e-05 | kPa | 320.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |

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|---|---|---|---|---|
| pvap | 3.11e-06 | kPa | 300.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 1.05e-05 | kPa | 310.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 2.46e-06 | kPa | 298.15 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 9.21e-05 | kPa | 330.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 2.42e-04 | kPa | 340.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 5.93e-04 | kPa | 350.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 1.36e-03 | kPa | 360.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |

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|---|---|---|---|---|
| pvap | 2.95e-03 | kPa | 370.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 6.07e-03 | kPa | 380.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.01 | kPa | 390.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.02 | kPa | 400.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.04 | kPa | 410.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.07 | kPa | 420.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.12 | kPa | 430.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |

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| pvap | 0.19 | kPa | 440.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.29 | kPa | 450.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.45 | kPa | 460.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.67 | kPa | 470.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 0.97 | kPa | 480.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 1.38 | kPa | 490.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| pvap | 1.93 | kPa | 500.00 | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |

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|---|---|---|---|---|
| pvap | 2.64 | kPa | 510.00 | 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 | 1.29338e+01 |
| Coeff. B | -4.38417e+03 |
| Coeff. C | -1.21066e+02 |
| Temperature range (K), min. | 467.74 |
| Temperature range (K), max. | 696.24 |

# Sources

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|---|---|
| **Thermochemistry of some alkylsubstituted anthracenes:** | https://www.doi.org/10.1016/j.jct.2005.06.001 |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C781431&Units=SI |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:** | https://www.doi.org/10.1021/je800300x |
| **Solubilities of Triptycene, 9-Phenylanthracene, 9,10-Dimethylanthracene, and 2-Methylanthracene in Pressurized Hot Water at Temperatures from 313 K to the Melting Point:** | https://www.doi.org/10.1021/je700447m |
| **Modified Watson Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |

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| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **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 |