# Anthracene, 9,10-dichloro-

**Other names:** 9,10-Dichloroanthracene
**Inchi:** InChI=1S/C14H8Cl2/c15-13-9-5-1-2-6-10(9)14(16)12-8-4-3-7-11(12)13/h1-8H
**InchiKey:** FKDIWXZNKAZCBY-UHFFFAOYSA-N
**Formula:** C14H8Cl2
**SMILES:** Clc1c2ccccc2c(Cl)c2ccccc12
**Mol. weight [g/mol]:** 247.12
**CAS:** 605-48-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 339.96 | kJ/mol | Joback Method |
| hf | 220.49 | kJ/mol | Joback Method |
| hfus | 27.32 | kJ/mol | Joback Method |
| hvap | 63.07 | kJ/mol | Joback Method |
| ie | 7.58 | eV | NIST Webbook |
| log10ws | -6.45 | | Crippen Method |
| logp | 5.300 | | Crippen Method |
| mcvol | 169.920 | ml/mol | McGowan Method |
| pc | 2890.51 | kPa | Joback Method |
| tb | 674.16 | K | Joback Method |
| tc | 935.50 | K | Joback Method |
| tf | 436.76 | K | Joback Method |
| vc | 0.653 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 437.30 | J/mol×K | 935.50 | Joback Method |
| cpg | 390.54 | J/mol×K | 717.72 | Joback Method |
| cpg | 401.34 | J/mol×K | 761.27 | Joback Method |
| cpg | 411.27 | J/mol×K | 804.83 | Joback Method |
| cpg | 420.48 | J/mol×K | 848.38 | Joback Method |
| cpg | 429.11 | J/mol×K | 891.94 | Joback Method |
| cpg | 378.73 | J/mol×K | 674.16 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005614 | Pa×s | 634.59 | Joback Method |
| dvisc | 0.0006403 | Pa×s | 595.03 | Joback Method |
| dvisc | 0.0007442 | Pa×s | 555.46 | Joback Method |
| dvisc | 0.0008851 | Pa×s | 515.89 | Joback Method |
| dvisc | 0.0010835 | Pa×s | 476.33 | Joback Method |
| dvisc | 0.0004998 | Pa×s | 674.16 | Joback Method |
| dvisc | 0.0013758 | Pa×s | 436.76 | Joback Method |
| hsubt | 113.90 ± 4.50 | kJ/mol | 346.00 | NIST Webbook |
| psub | 8.70e-06 | kPa | 344.30 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |
| psub | 1.44e-05 | kPa | 347.30 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |
| psub | 7.10e-06 | kPa | 341.70 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |
| psub | 1.72e-05 | kPa | 348.90 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |

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| psub | 3.70e-05 | kPa | 353.40 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |
| psub | 3.94e-05 | kPa | 353.60 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |
| psub | 3.74e-05 | kPa | 355.80 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |
| psub | 5.46e-05 | kPa | 357.90 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |
| psub | 8.47e-05 | kPa | 363.50 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |

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| psub | 7.79e-05 | kPa | 364.40 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |
| psub | 1.21e-04 | kPa | 367.50 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |
| psub | 1.64e-04 | kPa | 368.50 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |
| psub | 2.36e-04 | kPa | 376.00 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |
| psub | 5.70e-06 | kPa | 339.10 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |

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|---|---|---|---|---|---|
| psub | 4.70e-06 | kPa | 337.70 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |
| psub | 2.20e-06 | kPa | 330.90 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |
| psub | 2.00e-06 | kPa | 330.80 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |
| psub | 2.70e-07 | kPa | 316.00 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |
| psub | 1.27e-05 | kPa | 345.60 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique | |

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|---|---|---|---|---|
| psub | 1.67e-05 | kPa | 348.30 | The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C605481&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique:** | https://www.doi.org/10.1016/j.jct.2007.09.006 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

| | |
|---|---|
| **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 |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **psub:** | Sublimation pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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