

# Anthracene, 9,10-dichloro-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 9,10-Dichloroanthracene   |
| <b>Inchi:</b>               | InChI=1S/C14H8Cl2/c15-13-9-5-1-2-6-10(9)14(16)12-8-4-3-7-11(12)13/h1-8H |
| <b>InchiKey:</b>            | FKDIWXZNKAZCBBY-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C14H8Cl2  |
| <b>SMILES:</b>              | Clc1c2ccccc2c(Cl)c2ccccc12  |
| <b>Mol. weight [g/mol]:</b> | 247.12  |
| <b>CAS:</b>                 | 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           | 378.73 | J/molxK | 674.16          | Joback Method |
| cpg           | 390.54 | J/molxK | 717.72          | Joback Method |
| cpg           | 401.34 | J/molxK | 761.27          | Joback Method |
| cpg           | 411.27 | J/molxK | 804.83          | Joback Method |
| cpg           | 420.48 | J/molxK | 848.38          | Joback Method |
| cpg           | 429.11 | J/molxK | 891.94          | Joback Method |
| cpg           | 437.30 | J/molxK | 935.50          | Joback Method |

|       |               |        |        |   |
|-------|---------------|--------|--------|---|
| dvisc | 0.0013758     | Paxs   | 436.76 | Joback Method   |
| dvisc | 0.0010835     | Paxs   | 476.33 | Joback Method   |
| dvisc | 0.0008851     | Paxs   | 515.89 | Joback Method   |
| dvisc | 0.0007442     | Paxs   | 555.46 | Joback Method   |
| dvisc | 0.0006403     | Paxs   | 595.03 | Joback Method   |
| dvisc | 0.0005614     | Paxs   | 634.59 | Joback Method   |
| dvisc | 0.0004998     | Paxs   | 674.16 | Joback Method   |
| hsubt | 113.90 ± 4.50 | kJ/mol | 346.00 | NIST Webbook  |
| 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  | 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 | 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 |
| 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 | 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 | 1.27e-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 |
| 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 | 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 |
| 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 |
| 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 |
| 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 |
|------|----------|-----|--------|---|

## Sources

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

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hsubt:</b>   | Enthalpy of sublimation at a given temperature  |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>psub:</b>    | Sublimation pressure                            |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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