

# Dibenzo[ef,hi]naphtho[8,1,2-abc]coronene

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C36H16/c1-4-17-12-14-26-24-9-3-8-23-21-7-2-5-19-16-20-11-10-18-13-15-25-2 |
| <b>InchiKey:</b>            | KXAPPMQHUSIBDC-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C36H16   |
| <b>SMILES:</b>              | <chem>c1cc2ccc3c4ccccc5c6cccc7cc8ccc9ccc%10c(c1)c2c3c1c%10c9c8c(c76)c1c54</chem>   |
| <b>Mol. weight [g/mol]:</b> | 448.51   |
| <b>CAS:</b>                 | 128395-03-9  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 1315.68 | kJ/mol  | Joback Method  |
| hf            | 1030.33 | kJ/mol  | Joback Method  |
| hfus          | 64.62   | kJ/mol  | Joback Method  |
| hvap          | 117.18  | kJ/mol  | Joback Method  |
| log10ws       | -16.59  |         | Crippen Method |
| logp          | 10.408  |         | Crippen Method |
| mcvol         | 321.240 | ml/mol  | McGowan Method |
| pc            | 1655.15 | kPa     | Joback Method  |
| tb            | 1245.88 | K       | Joback Method  |
| tc            | 1533.31 | K       | Joback Method  |
| tf            | 992.98  | K       | Joback Method  |
| vc            | 1.313   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1158.15   | J/molxK | 1245.88         | Joback Method |
| cpg           | 1538.20   | J/molxK | 1485.41         | Joback Method |
| cpg           | 1442.05   | J/molxK | 1437.50         | Joback Method |
| cpg           | 1356.83   | J/molxK | 1389.60         | Joback Method |
| cpg           | 1281.69   | J/molxK | 1341.69         | Joback Method |
| cpg           | 1215.75   | J/molxK | 1293.79         | Joback Method |
| cpg           | 1646.14   | J/molxK | 1533.31         | Joback Method |
| dvisc         | 2.2745745 | Paxs    | 1245.88         | Joback Method |
| dvisc         | 2.1893823 | Paxs    | 1203.73         | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 2.1015508 | Paxs | 1161.58 | Joback Method |
| dvisc | 2.0110325 | Paxs | 1119.43 | Joback Method |
| dvisc | 1.9177944 | Paxs | 1077.28 | Joback Method |
| dvisc | 1.8218221 | Paxs | 1035.13 | Joback Method |
| dvisc | 1.7231260 | Paxs | 992.98  | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C128395039&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C128395039&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                       |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>                           |

## 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>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <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>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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