

# Tribenzo[b,g,k]chrysene

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C30H18/c1-2-8-20-16-27-23(15-19(20)7-1)13-14-26-29-18-22-10-4-3-9-21(22) |
| <b>InchiKey:</b>            | XXHBWGDULJLIOR-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C30H18  |
| <b>SMILES:</b>              | <chem>c1ccc2cc3c(ccc4c5cc6ccccc6cc5c5ccccc5c34)cc2c1</chem>                       |
| <b>Mol. weight [g/mol]:</b> | 378.46  |
| <b>CAS:</b>                 | 115747-46-1   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 905.88  | kJ/mol               | Joback Method  |
| hf            | 663.07  | kJ/mol               | Joback Method  |
| hfus          | 47.67   | kJ/mol               | Joback Method  |
| hvap          | 97.80   | kJ/mol               | Joback Method  |
| log10ws       | -12.30  |                      | Crippen Method |
| logp          | 8.606   |                      | Crippen Method |
| mvol          | 293.040 | ml/mol               | McGowan Method |
| pc            | 1777.34 | kPa                  | Joback Method  |
| tb            | 1051.26 | K                    | Joback Method  |
| tc            | 1330.47 | K                    | Joback Method  |
| tf            | 713.08  | K                    | Joback Method  |
| vc            | 1.139   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 909.76    | J/molxK | 1051.26         | Joback Method |
| cpg           | 929.78    | J/molxK | 1097.80         | Joback Method |
| cpg           | 951.06    | J/molxK | 1144.33         | Joback Method |
| cpg           | 974.05    | J/molxK | 1190.87         | Joback Method |
| cpg           | 999.18    | J/molxK | 1237.40         | Joback Method |
| cpg           | 1026.90   | J/molxK | 1283.94         | Joback Method |
| cpg           | 1057.66   | J/molxK | 1330.47         | Joback Method |
| dvisc         | 0.0046199 | Paxs    | 713.08          | Joback Method |
| dvisc         | 0.0041148 | Paxs    | 769.44          | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0037234 | Paxs | 825.81  | Joback Method |
| dvisc | 0.0034125 | Paxs | 882.17  | Joback Method |
| dvisc | 0.0031604 | Paxs | 938.53  | Joback Method |
| dvisc | 0.0029526 | Paxs | 994.90  | Joback Method |
| dvisc | 0.0027786 | Paxs | 1051.26 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C115747461&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C115747461&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>                                       |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>mccvol:</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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