# 4H-Cyclopenta[def]phenanthrenequinone

**Inchi:** InChI=1S/C15H8O2/c16-14-10-5-1-3-8-7-9-4-2-6-11(15(14)17)13(9)12(8)10/h1-6H,7H2
**InchiKey:** AHDICIQOAZDBEN-UHFFFAOYSA-N
**Formula:** C15H8O2
**SMILES:** O=C1C(=O)c2cccc3c2-c2c(cccc21)C3
**Mol. weight [g/mol]:** 220.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 189.76 | kJ/mol | Joback Method |
| hf | 3.61 | kJ/mol | Joback Method |
| hfus | 20.58 | kJ/mol | Joback Method |
| hvap | 64.61 | kJ/mol | Joback Method |
| log10ws | -4.80 | | Crippen Method |
| logp | 2.637 | | Crippen Method |
| mcvol | 156.110 | ml/mol | McGowan Method |
| pc | 3322.01 | kPa | Joback Method |
| rinpol | 342.64 | | NIST Webbook |
| rinpol | 2195.00 | | NIST Webbook |
| tb | 761.53 | K | Joback Method |
| tc | 1031.86 | K | Joback Method |
| tf | 553.09 | K | Joback Method |
| vc | 0.614 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 424.33 | J/mol×K | 761.53 | Joback Method |
| cpg | 436.98 | J/mol×K | 806.59 | Joback Method |
| cpg | 448.77 | J/mol×K | 851.64 | Joback Method |
| cpg | 459.82 | J/mol×K | 896.70 | Joback Method |
| cpg | 470.26 | J/mol×K | 941.75 | Joback Method |
| cpg | 480.22 | J/mol×K | 986.81 | Joback Method |
| cpg | 489.83 | J/mol×K | 1031.86 | Joback Method |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R553109&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |