# Cyclopropa[c]2h-1-benzopyran,3,4-dihydro-4-phe

**Inchi:** InChI=1S/C16H14O/c1-2-6-12(7-3-1)16-10-13(16)11-17-15-9-5-4-8-14(15)16/h1-9,13H,1
**InchiKey:** WARAYOPBTKJQFK-UHFFFAOYSA-N
**Formula:** C16H14O
**SMILES:** c1ccc(C23CC2COc2ccccc23)cc1
**Mol. weight [g/mol]:** 222.28
**CAS:** 6719-35-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 341.02 | kJ/mol | Joback Method |
| hf | 123.02 | kJ/mol | Joback Method |
| hfus | 24.94 | kJ/mol | Joback Method |
| hvap | 59.44 | kJ/mol | Joback Method |
| log10ws | -3.75 | | Crippen Method |
| logp | 3.385 | | Crippen Method |
| mcvol | 172.930 | ml/mol | McGowan Method |
| pc | 2966.57 | kPa | Joback Method |
| tb | 660.22 | K | Joback Method |
| tc | 923.82 | K | Joback Method |
| tf | 425.31 | K | Joback Method |
| vc | 0.656 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 468.51 | J/mol×K | 660.22 | Joback Method |
| cpg | 485.91 | J/mol×K | 704.15 | Joback Method |
| cpg | 502.08 | J/mol×K | 748.09 | Joback Method |
| cpg | 517.38 | J/mol×K | 792.02 | Joback Method |
| cpg | 532.18 | J/mol×K | 835.95 | Joback Method |
| cpg | 546.85 | J/mol×K | 879.89 | Joback Method |
| cpg | 561.75 | J/mol×K | 923.82 | 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=C6719353&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |