# cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, 3-methoxy

**Inchi:** InChI=1S/C16H16O3/c1-16(18)14-6-4-3-5-11(14)13-9-10(19-2)7-8-12(13)15(16)17/h3-9,

**InchiKey:** ISRUVUJGAGZJCM-CVEARBPZSA-N

**Formula:** C16H16O3

**SMILES:** COc1ccc2c(c1)-c1ccccc1C(C)(O)C2O

**Mol. weight [g/mol]:** 256.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -39.22 | kJ/mol | Joback Method |
| hf | -297.74 | kJ/mol | Joback Method |
| hfus | 28.48 | kJ/mol | Joback Method |
| hvap | 91.80 | kJ/mol | Joback Method |
| log10ws | -4.43 | | Crippen Method |
| logp | 2.617 | | Crippen Method |
| mcvol | 195.530 | ml/mol | McGowan Method |
| pc | 2912.39 | kPa | Joback Method |
| rinpol | 2350.00 | | NIST Webbook |
| tb | 838.60 | K | Joback Method |
| tc | 1053.42 | K | Joback Method |
| tf | 545.47 | K | Joback Method |
| vc | 0.734 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 588.06 | J/mol×K | 838.60 | Joback Method |
| cpg | 600.97 | J/mol×K | 874.40 | Joback Method |
| cpg | 613.78 | J/mol×K | 910.21 | Joback Method |
| cpg | 626.63 | J/mol×K | 946.01 | Joback Method |
| cpg | 639.66 | J/mol×K | 981.82 | Joback Method |
| cpg | 653.03 | J/mol×K | 1017.62 | Joback Method |
| cpg | 666.86 | J/mol×K | 1053.42 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=R109514&Units=SI |

# Legend

| | |
|---|---|
| **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 |