# Benzo[c]phenanthrene

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|---|---|
| **Other names:** | 3,4-Benzophenanthrene |
| | Benzo-3,4-phenanthrene |
| | Tetrahelicene |
| | 3,4-Benzphenanthrene |
| **Inchi:** | InChI=1S/C18H12/c1-3-7-16-13(5-1)9-11-15-12-10-14-6-2-4-8-17(14)18(15)16/h1-12H |
| **InchiKey:** | TUAHORSUHVUKBD-UHFFFAOYSA-N |
| **Formula:** | C18H12 |
| **SMILES:** | c1ccc2c(c1)ccc1ccc3ccccc3c12 |
| **Mol. weight [g/mol]:** | 228.29 |
| **CAS:** | 195-19-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -8983.00 ± 1.90 | kJ/mol | NIST Webbook |
| ea | 0.55 ± 0.01 | eV | NIST Webbook |
| ea | 0.33 | eV | NIST Webbook |
| gf | 513.78 | kJ/mol | Joback Method |
| hf | 291.20 | kJ/mol | NIST Webbook |
| hfs | 184.90 ± 3.00 | kJ/mol | NIST Webbook |
| hfus | 26.70 | kJ/mol | Joback Method |
| hsub | 106.30 | kJ/mol | NIST Webbook |
| hsub | 106.00 | kJ/mol | NIST Webbook |
| hvap | 64.18 | kJ/mol | Joback Method |
| ie | 7.62 | eV | NIST Webbook |
| ie | 7.76 | eV | NIST Webbook |
| ie | 7.86 | eV | NIST Webbook |
| ie | 7.60 | eV | NIST Webbook |
| ie | 7.60 ± 0.02 | eV | NIST Webbook |
| log10ws | -6.88 | | Crippen Method |
| logp | 5.146 | | Crippen Method |
| mcvol | 182.340 | ml/mol | McGowan Method |
| pc | 2741.15 | kPa | Joback Method |
| rinpol | 2390.00 | | NIST Webbook |
| rinpol | 391.24 | | NIST Webbook |
| rinpol | 391.39 | | NIST Webbook |
| rinpol | 390.90 | | NIST Webbook |
| rinpol | 2400.20 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 390.57 | | NIST Webbook |
| rinpol | 391.07 | | NIST Webbook |
| rinpol | 391.24 | | NIST Webbook |
| rinpol | 2427.00 | | NIST Webbook |
| rinpol | 391.10 | | NIST Webbook |
| rinpol | 389.52 | | NIST Webbook |
| rinpol | 388.58 | | NIST Webbook |
| rinpol | 389.97 | | NIST Webbook |
| rinpol | 390.27 | | NIST Webbook |
| rinpol | 391.39 | | NIST Webbook |
| rinpol | 2400.20 | | NIST Webbook |
| rinpol | 2390.00 | | NIST Webbook |
| rinpol | 391.07 | | NIST Webbook |
| rinpol | 394.30 | | NIST Webbook |
| rinpol | 391.12 | | NIST Webbook |
| rinpol | 390.89 | | NIST Webbook |
| rinpol | 391.07 | | NIST Webbook |
| rinpol | 391.11 | | NIST Webbook |
| rinpol | 391.30 | | NIST Webbook |
| rinpol | 2400.00 | | NIST Webbook |
| rinpol | 2390.00 | | NIST Webbook |
| rinpol | 2400.00 | | NIST Webbook |
| rinpol | 390.57 | | NIST Webbook |
| rinpol | 389.36 | | NIST Webbook |
| rinpol | 2427.00 | | NIST Webbook |
| tb | 704.82 | K | Joback Method |
| tc | 968.39 | K | Joback Method |
| tf | 342.00 ± 1.00 | K | NIST Webbook |
| tf | 334.80 ± 0.80 | K | NIST Webbook |
| tf | 341.00 ± 1.00 | K | NIST Webbook |
| vc | 0.702 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 468.00 | J/mol×K | 704.82 | Joback Method |
| cpg | 482.86 | J/mol×K | 748.75 | Joback Method |
| cpg | 496.51 | J/mol×K | 792.68 | Joback Method |
| cpg | 509.15 | J/mol×K | 836.61 | Joback Method |
| cpg | 521.02 | J/mol×K | 880.54 | Joback Method |
| cpg | 532.31 | J/mol×K | 924.47 | Joback Method |

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|---|---|---|---|---|
| cpg | 543.24 | J/mol×K | 968.39 | Joback Method |
| dvisc | 0.0011669 | Pa×s | 529.73 | Joback Method |
| dvisc | 0.0013935 | Pa×s | 485.95 | Joback Method |
| dvisc | 0.0017235 | Pa×s | 442.18 | Joback Method |
| dvisc | 0.0010040 | Pa×s | 573.50 | Joback Method |
| dvisc | 0.0008825 | Pa×s | 617.27 | Joback Method |
| dvisc | 0.0007890 | Pa×s | 661.05 | Joback Method |
| dvisc | 0.0007153 | Pa×s | 704.82 | Joback Method |
| hfust | 15.50 | kJ/mol | 339.20 | NIST Webbook |
| hfust | 16.32 | kJ/mol | 334.70 | NIST Webbook |
| hfust | 16.32 | kJ/mol | 334.70 | NIST Webbook |
| hsubt | 106.00 | kJ/mol | 293.00 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C195197&Units=SI
**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

# Legend

**chs:** Standard solid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**ea:** Electron affinity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfs:** Solid phase enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hfust:** Enthalpy of fusion at a given temperature
**hsub:** Enthalpy of sublimation at standard conditions
**hsubt:** Enthalpy of sublimation at a given temperature
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient

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