# 3-Hydroxybenz[a]anthracene

**Inchi:** InChI=1S/C18H12O/c19-16-7-8-17-15(10-16)6-5-14-9-12-3-1-2-4-13(12)11-18(14)17/h1-
**InchiKey:** MRRWKFVZIOCJBS-UHFFFAOYSA-N
**Formula:** C18H12O
**SMILES:** Oc1ccc2c(ccc3cc4ccccc4cc32)c1
**Mol. weight [g/mol]:** 244.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 359.16 | kJ/mol | Joback Method |
| hf | 194.64 | kJ/mol | Joback Method |
| hfus | 32.48 | kJ/mol | Joback Method |
| hvap | 77.20 | kJ/mol | Joback Method |
| log10ws | -6.43 | | Crippen Method |
| logp | 4.852 | | Crippen Method |
| mcvol | 188.210 | ml/mol | McGowan Method |
| pc | 3224.64 | kPa | Joback Method |
| rinpol | 2871.00 | | NIST Webbook |
| rinpol | 2871.00 | | NIST Webbook |
| tb | 785.44 | K | Joback Method |
| tc | 1054.46 | K | Joback Method |
| tf | 553.90 | K | Joback Method |
| vc | 0.667 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 513.18 | J/mol×K | 785.44 | Joback Method |
| cpg | 526.28 | J/mol×K | 830.28 | Joback Method |
| cpg | 538.83 | J/mol×K | 875.11 | Joback Method |
| cpg | 551.14 | J/mol×K | 919.95 | Joback Method |
| cpg | 563.49 | J/mol×K | 964.79 | Joback Method |
| cpg | 576.20 | J/mol×K | 1009.62 | Joback Method |
| cpg | 589.56 | J/mol×K | 1054.46 | Joback Method |
| dvisc | 0.0003579 | Pa×s | 553.90 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002356 | Pa×s | 592.49 | Joback Method |
| dvisc | 0.0001632 | Pa×s | 631.08 | Joback Method |
| dvisc | 0.0001180 | Pa×s | 669.67 | Joback Method |
| dvisc | 0.0000883 | Pa×s | 708.26 | Joback Method |
| dvisc | 0.0000681 | Pa×s | 746.85 | Joback Method |
| dvisc | 0.0000539 | Pa×s | 785.44 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R588615&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

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |

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