# 7-Butylbenz[a]anthracene

**Inchi:** InChI=1S/C22H20/c1-2-3-10-20-19-12-7-5-9-17(19)15-22-18-11-6-4-8-16(18)13-14-21(20
**InchiKey:** BIOVWIBRVOHDTA-UHFFFAOYSA-N
**Formula:** C22H20
**SMILES:** CCCCc1c2ccccc2cc2c1ccc1ccccc12
**Mol. weight [g/mol]:** 284.39
**CAS:** 18868-65-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 537.83 | kJ/mol | Joback Method |
| hf | 277.92 | kJ/mol | Joback Method |
| hfus | 36.67 | kJ/mol | Joback Method |
| hvap | 73.75 | kJ/mol | Joback Method |
| log10ws | -8.52 | | Crippen Method |
| logp | 6.489 | | Crippen Method |
| mcvol | 238.700 | ml/mol | McGowan Method |
| pc | 1875.65 | kPa | Joback Method |
| tb | 801.32 | K | Joback Method |
| tc | 1043.67 | K | Joback Method |
| tf | 499.78 | K | Joback Method |
| vc | 0.925 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 681.57 | J/mol×K | 801.32 | Joback Method |
| cpg | 697.89 | J/mol×K | 841.71 | Joback Method |
| cpg | 713.25 | J/mol×K | 882.10 | Joback Method |
| cpg | 727.85 | J/mol×K | 922.50 | Joback Method |
| cpg | 741.85 | J/mol×K | 962.89 | Joback Method |
| cpg | 755.42 | J/mol×K | 1003.28 | Joback Method |
| cpg | 768.76 | J/mol×K | 1043.67 | Joback Method |
| dvisc | 0.0015546 | Pa×s | 499.78 | Joback Method |
| dvisc | 0.0012104 | Pa×s | 550.04 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0009827 | Pa×s | 600.29 | Joback Method |
| dvisc | 0.0008240 | Pa×s | 650.55 | Joback Method |
| dvisc | 0.0007086 | Pa×s | 700.81 | Joback Method |
| dvisc | 0.0006218 | Pa×s | 751.06 | Joback Method |
| dvisc | 0.0005546 | Pa×s | 801.32 | Joback Method |

# Sources

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|---|---|
| **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=C18868650&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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |