# Benz[a]anthracene, 1,12-dimethyl-

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|---|---|
| **Other names:** | 1,12-Dimethylbenz[a]anthracene |
| | 1',9-Dimethyl-1,2-benzanthracene |
| | Benz[b]anthracene, 7,12-dimethyl |
| | 1,12-Dimethylbenzo[a]anthracene |
| **Inchi:** | InChI=1S/C20H16/c1-13-6-5-8-15-10-11-17-12-16-7-3-4-9-18(16)14(2)20(17)19(13)15/h3 |
| **InchiKey:** | XDOAGYHDDFESMV-UHFFFAOYSA-N |
| **Formula:** | C20H16 |
| **SMILES:** | Cc1cccc2ccc3cc4ccccc4c(C)c3c12 |
| **Mol. weight [g/mol]:** | 256.34 |
| **CAS:** | 313-74-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -10295.80 ± 2.00 | kJ/mol | NIST Webbook |
| gf | 511.36 | kJ/mol | Joback Method |
| hf | 307.73 | kJ/mol | Joback Method |
| hfs | 138.90 ± 2.80 | kJ/mol | NIST Webbook |
| hfus | 31.10 | kJ/mol | Joback Method |
| hvap | 69.96 | kJ/mol | Joback Method |
| log10ws | -7.84 | | Crippen Method |
| logp | 5.763 | | Crippen Method |
| mcvol | 210.520 | ml/mol | McGowan Method |
| pc | 2200.01 | kPa | Joback Method |
| rinpol | 436.43 | | NIST Webbook |
| rinpol | 436.82 | | NIST Webbook |
| rinpol | 440.30 | | NIST Webbook |
| rinpol | 2822.00 | | NIST Webbook |
| rinpol | 2822.00 | | NIST Webbook |
| rinpol | 436.82 | | NIST Webbook |
| tb | 760.54 | K | Joback Method |
| tc | 1013.66 | K | Joback Method |
| tf | 489.76 | K | Joback Method |
| vc | 0.814 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 639.81 | J/mol×K | 971.47 | Joback Method |
| cpg | 600.62 | J/mol×K | 844.91 | Joback Method |
| cpg | 586.13 | J/mol×K | 802.73 | Joback Method |
| cpg | 570.63 | J/mol×K | 760.54 | Joback Method |
| cpg | 614.28 | J/mol×K | 887.10 | Joback Method |
| cpg | 652.05 | J/mol×K | 1013.66 | Joback Method |
| cpg | 627.28 | J/mol×K | 929.28 | Joback Method |
| dvisc | 0.0014862 | Pa×s | 489.76 | Joback Method |
| dvisc | 0.0006539 | Pa×s | 760.54 | Joback Method |
| dvisc | 0.0007181 | Pa×s | 715.41 | Joback Method |
| dvisc | 0.0007987 | Pa×s | 670.28 | Joback Method |
| dvisc | 0.0009019 | Pa×s | 625.15 | Joback Method |
| dvisc | 0.0010381 | Pa×s | 580.02 | Joback Method |
| dvisc | 0.0012234 | Pa×s | 534.89 | Joback Method |
| hsubt | 135.00 | kJ/mol | 384.50 | NIST Webbook |
| hvapt | 112.90 | kJ/mol | 402.00 | NIST Webbook |
| hvapt | 88.90 | kJ/mol | 398.00 | NIST Webbook |
| hvapt | 107.80 | kJ/mol | 387.50 | NIST Webbook |

# 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=C313746&Units=SI

# Legend

**chs:** Standard solid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation

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|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |