# Benz(a)anthracene, 7-ethyl-12-methyl-

**Other names:** 7-Ethyl-12-methylbenz(a)anthracene
**Inchi:** InChI=1S/C21H18/c1-3-16-19-11-7-6-9-17(19)14(2)21-18-10-5-4-8-15(18)12-13-20(16)21
**InchiKey:** KGHAOMPXHGIHAL-UHFFFAOYSA-N
**Formula:** C21H18
**SMILES:** CCc1c2ccccc2c(C)c2c1ccc1ccccc12
**Mol. weight [g/mol]:** 270.37
**CAS:** 16354-50-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 519.78 | kJ/mol | Joback Method |
| hf | 287.09 | kJ/mol | Joback Method |
| hfus | 33.69 | kJ/mol | Joback Method |
| hvap | 72.18 | kJ/mol | Joback Method |
| log10ws | -8.16 | | Crippen Method |
| logp | 6.017 | | Crippen Method |
| mcvol | 224.610 | ml/mol | McGowan Method |
| pc | 2014.51 | kPa | Joback Method |
| tb | 783.42 | K | Joback Method |
| tc | 1031.24 | K | Joback Method |
| tf | 501.03 | K | Joback Method |
| vc | 0.870 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 625.02 | J/mol×K | 783.42 | Joback Method |
| cpg | 696.57 | J/mol×K | 989.94 | Joback Method |
| cpg | 683.49 | J/mol×K | 948.64 | Joback Method |
| cpg | 669.98 | J/mol×K | 907.33 | Joback Method |
| cpg | 655.84 | J/mol×K | 866.03 | Joback Method |
| cpg | 640.91 | J/mol×K | 824.72 | Joback Method |
| cpg | 709.36 | J/mol×K | 1031.24 | Joback Method |
| dvisc | 0.0006104 | Pa×s | 783.42 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0006744 | Pa×s | 736.36 | Joback Method |
| dvisc | 0.0007555 | Pa×s | 689.29 | Joback Method |
| dvisc | 0.0008604 | Pa×s | 642.23 | Joback Method |
| dvisc | 0.0010003 | Pa×s | 595.16 | Joback Method |
| dvisc | 0.0011934 | Pa×s | 548.10 | Joback Method |
| dvisc | 0.0014719 | Pa×s | 501.03 | Joback Method |

# Sources

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|---|---|
| **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=C16354500&Units=SI |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |