

Benz[a]anthracene, 11-methyl-

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|-----------------------------|--|
| Other names: | 11-Methylbenz[a]anthracene 8-Methyl-1,2-benzanthracene Benzo[a]anthracene, 11-methyl |
| Inchi: | InChI=1S/C19H14/c1-13-5-4-7-15-11-16-10-9-14-6-2-3-8-17(14)19(16)12-18(13)15/h2-12 |
| InchiKey: | ARHCZXQENFEAFA-UHFFFAOYSA-N |
| Formula: | C19H14 |
| SMILES: | Cc1cccc2cc3ccc4ccccc4c3cc12 |
| Mol. weight [g/mol]: | 242.31 |
| CAS: | 6111-78-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|---------|----------------|
| gf | 512.57 | kJ/mol | Joback Method |
| hf | 339.84 | kJ/mol | Joback Method |
| hfus | 28.90 | kJ/mol | Joback Method |
| hvap | 67.07 | kJ/mol | Joback Method |
| ie | 7.30 ± 0.03 | eV | NIST Webbook |
| log10ws | -7.36 | | Crippen Method |
| logp | 5.455 | | Crippen Method |
| mcvol | 196.430 | ml/mol | McGowan Method |
| pc | 2448.32 | kPa | Joback Method |
| rinpol | 412.72 | | NIST Webbook |
| rinpol | 412.88 | | NIST Webbook |
| rinpol | 412.72 | | NIST Webbook |
| rinpol | 412.88 | | NIST Webbook |
| rinpol | 412.05 | | NIST Webbook |
| rinpol | 412.72 | | NIST Webbook |
| tb | 732.68 | K | Joback Method |
| tc | 990.82 | K | Joback Method |
| tf | 465.97 | K | Joback Method |
| vc | 0.757 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 518.66 | J/mol×K | 732.68 | Joback Method |
| cpg | 533.84 | J/mol×K | 775.70 | Joback Method |
| cpg | 547.92 | J/mol×K | 818.73 | Joback Method |
| cpg | 561.09 | J/mol×K | 861.75 | Joback Method |
| cpg | 573.55 | J/mol×K | 904.77 | Joback Method |
| cpg | 585.49 | J/mol×K | 947.80 | Joback Method |
| cpg | 597.11 | J/mol×K | 990.82 | Joback Method |
| dvisc | 0.0016009 | Paxs | 465.97 | Joback Method |
| dvisc | 0.0013067 | Paxs | 510.42 | Joback Method |
| dvisc | 0.0011019 | Paxs | 554.87 | Joback Method |
| dvisc | 0.0009529 | Paxs | 599.33 | Joback Method |
| dvisc | 0.0008408 | Paxs | 643.78 | Joback Method |
| dvisc | 0.0007540 | Paxs | 688.23 | Joback Method |
| dvisc | 0.0006851 | Paxs | 732.68 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6111780&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| ie: | Ionization energy |
| 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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