# 5H-Benzocycloheptene, 5-phenyl-6,7,8,9-tetrahydro-

**Inchi:** InChI=1S/C17H18/c1-2-8-14(9-3-1)16-12-6-4-10-15-11-5-7-13-17(15)16/h1-3,5,7-9,11,13

**InchiKey:** UYQXAXXXMIEYGP-UHFFFAOYSA-N

**Formula:** C17H18

**SMILES:** c1ccc(C2CCCCc3ccccc32)cc1

**Mol. weight [g/mol]:** 222.32

**CAS:** 35068-34-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 344.00 | kJ/mol | Joback Method |
| hf | 127.86 | kJ/mol | Joback Method |
| hfus | 21.41 | kJ/mol | Joback Method |
| hvap | 58.91 | kJ/mol | Joback Method |
| log10ws | -5.07 | | Crippen Method |
| logp | 4.545 | | Crippen Method |
| mcvol | 192.010 | ml/mol | McGowan Method |
| pc | 2443.48 | kPa | Joback Method |
| tb | 661.98 | K | Joback Method |
| tc | 921.39 | K | Joback Method |
| tf | 357.61 | K | Joback Method |
| vc | 0.713 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 514.22 | J/mol×K | 661.98 | Joback Method |
| cpg | 604.18 | J/mol×K | 878.15 | Joback Method |
| cpg | 589.29 | J/mol×K | 834.92 | Joback Method |
| cpg | 572.97 | J/mol×K | 791.68 | Joback Method |
| cpg | 555.10 | J/mol×K | 748.45 | Joback Method |
| cpg | 535.56 | J/mol×K | 705.21 | Joback Method |
| cpg | 617.78 | J/mol×K | 921.39 | Joback Method |
| dvisc | 0.0001945 | Pa×s | 661.98 | Joback Method |
| dvisc | 0.0002449 | Pa×s | 611.25 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003215 | Pa×s | 560.52 | Joback Method |
| dvisc | 0.0004456 | Pa×s | 509.80 | Joback Method |
| dvisc | 0.0006636 | Pa×s | 459.07 | Joback Method |
| dvisc | 0.0010911 | Pa×s | 408.34 | Joback Method |
| dvisc | 0.0020660 | Pa×s | 357.61 | Joback Method |

# Sources

| | |
|---|---|
| **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=C35068349&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |