# Pentalene, octahydro-, cis-

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|---|---|
| **Other names:** | (Z)-Bicyclo[3.3.0]octane |
| | Bicyclo[3.3.0]octane |
| | Bicyclo[3.3.0]octane (cis) |
| | Octahydropentalene, (Z)- |
| | cis-Bicyclo[3.3.0]octane |
| | cis-Octahydropentalene |
| **Inchi:** | InChI=1S/C8H14/c1-3-7-5-2-6-8(7)4-1/h7-8H,1-6H2/t7-,8+ |
| **InchiKey:** | AEBWATHAIVJLTA-OCAPTIKFSA-N |
| **Formula:** | C8H14 |
| **SMILES:** | C1CC2CCCC2C1 |
| **Mol. weight [g/mol]:** | 110.20 |
| **CAS:** | 1755-05-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -4968.00 ± 1.00 | kJ/mol | NIST Webbook |
| chl | -5016.00 ± 2.80 | kJ/mol | NIST Webbook |
| chl | -5013.00 ± 1.00 | kJ/mol | NIST Webbook |
| gf | 113.78 | kJ/mol | Joback Method |
| hf | -93.00 ± 2.00 | kJ/mol | NIST Webbook |
| hfl | -136.00 ± 1.00 | kJ/mol | NIST Webbook |
| hfus | 8.55 | kJ/mol | Joback Method |
| hvap | 43.00 | kJ/mol | NIST Webbook |
| hvap | 43.10 ± 0.80 | kJ/mol | NIST Webbook |
| hvap | 43.10 ± 0.80 | kJ/mol | NIST Webbook |
| log10ws | -2.48 | | Crippen Method |
| logp | 2.587 | | Crippen Method |
| mcvol | 101.860 | ml/mol | McGowan Method |
| pc | 3560.02 | kPa | Joback Method |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 865.00 | | NIST Webbook |
| rinpol | 869.00 | | NIST Webbook |
| rinpol | 874.00 | | NIST Webbook |
| rinpol | 863.00 | | NIST Webbook |
| rinpol | 891.00 | | NIST Webbook |
| rinpol | 858.00 | | NIST Webbook |
| rinpol | 859.90 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 865.20 | | NIST Webbook |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 858.00 | | NIST Webbook |
| rinpol | 870.00 | | NIST Webbook |
| tb | 409.00 ± 3.00 | K | NIST Webbook |
| tb | 409.40 ± 2.00 | K | NIST Webbook |
| tb | 409.00 ± 3.00 | K | NIST Webbook |
| tb | 408.00 ± 2.00 | K | NIST Webbook |
| tb | 410.28 ± 0.20 | K | NIST Webbook |
| tc | 614.38 | K | Joback Method |
| tf | 224.00 ± 8.00 | K | NIST Webbook |
| tf | 223.82 ± 0.20 | K | NIST Webbook |
| tf | 224.00 ± 8.00 | K | NIST Webbook |
| vc | 0.382 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 292.95 | J/mol×K | 614.38 | Joback Method |
| cpg | 279.71 | J/mol×K | 579.39 | Joback Method |
| cpg | 265.55 | J/mol×K | 544.41 | Joback Method |
| cpg | 250.43 | J/mol×K | 509.42 | Joback Method |
| cpg | 234.29 | J/mol×K | 474.43 | Joback Method |
| cpg | 217.06 | J/mol×K | 439.45 | Joback Method |
| cpg | 198.70 | J/mol×K | 404.46 | Joback Method |
| cpl | 212.40 | J/mol×K | 308.00 | NIST Webbook |
| dvisc | 0.0004754 | Pa×s | 404.46 | Joback Method |
| dvisc | 0.0013767 | Pa×s | 208.76 | Joback Method |
| dvisc | 0.0005251 | Pa×s | 371.84 | Joback Method |
| dvisc | 0.0005912 | Pa×s | 339.23 | Joback Method |
| dvisc | 0.0006827 | Pa×s | 306.61 | Joback Method |
| dvisc | 0.0008158 | Pa×s | 273.99 | Joback Method |
| dvisc | 0.0010230 | Pa×s | 241.38 | Joback Method |
| hvapt | 41.50 ± 0.40 | kJ/mol | 318.00 | NIST Webbook |
| hvapt | 42.00 | kJ/mol | 308.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.45388e+01 |
| Coeff. B | -3.70158e+03 |
| Coeff. C | -4.15750e+01 |
| Temperature range (K), min. | 298.00 |
| Temperature range (K), max. | 442.73 |

# 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=C1755051&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **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 |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |

**tf:** Normal melting (fusion) point

**vc:** Critical Volume