# 1,6-Heptadiyne

**Other names:** hepta-1,6-diyne
**Inchi:** InChI=1S/C7H8/c1-3-5-7-6-4-2/h1-2H,5-7H2
**InchiKey:** RSPZSDWVQWRAEF-UHFFFAOYSA-N
**Formula:** C7H8
**SMILES:** C#CCCCC#C
**Mol. weight [g/mol]:** 92.14
**CAS:** 2396-63-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 454.20 | kJ/mol | Joback Method |
| hf | 395.99 | kJ/mol | Joback Method |
| hfus | 19.84 | kJ/mol | Joback Method |
| hvap | 30.89 | kJ/mol | Joback Method |
| ie | 9.85 ± 0.01 | eV | NIST Webbook |
| ie | 9.85 ± 0.01 | eV | NIST Webbook |
| log10ws | -2.34 | | Crippen Method |
| logp | 1.423 | | Crippen Method |
| mcvol | 92.290 | ml/mol | McGowan Method |
| pc | 3935.71 | kPa | Joback Method |
| rinpol | 663.00 | | NIST Webbook |
| rinpol | 664.00 | | NIST Webbook |
| rinpol | 664.00 | | NIST Webbook |
| rinpol | 664.00 | | NIST Webbook |
| tb | 385.20 ± 3.00 | K | NIST Webbook |
| tb | 384.65 ± 0.30 | K | NIST Webbook |
| tb | 385.20 | K | NIST Webbook |
| tc | 528.12 | K | Joback Method |
| tf | 188.31 ± 0.60 | K | NIST Webbook |
| vc | 0.351 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 151.52 | J/mol×K | 339.80 | Joback Method |
| cpg | 160.13 | J/mol×K | 371.19 | Joback Method |
| cpg | 168.29 | J/mol×K | 402.57 | Joback Method |
| cpg | 176.02 | J/mol×K | 433.96 | Joback Method |
| cpg | 183.34 | J/mol×K | 465.35 | Joback Method |
| cpg | 190.28 | J/mol×K | 496.73 | Joback Method |
| cpg | 196.85 | J/mol×K | 528.12 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 381.00 | K | 1.60 | NIST Webbook |
| tbrp | 393.00 | K | 8.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.63105e+01 |
| Coeff. B | -3.94000e+03 |
| Coeff. C | -4.82220e+01 |
| Temperature range (K), min. | 294.12 |
| Temperature range (K), max. | 406.44 |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2396636&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**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

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |