# Hex-3-en-1,5-diyne

**Inchi:** InChI=1S/C6H4/c1-3-5-6-4-2/h1-2,5-6H
**InchiKey:** KIWAUQFHKHLABA-UHFFFAOYSA-N
**Formula:** C6H4
**SMILES:** C#CC=CC#C
**Mol. weight [g/mol]:** 76.10
**CAS:** 6929-94-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 526.00 | kJ/mol | Joback Method |
| hf | 533.85 | kJ/mol | Joback Method |
| hfus | 17.45 | kJ/mol | Joback Method |
| hvap | 28.62 | kJ/mol | Joback Method |
| ie | 9.60 ± 0.20 | eV | NIST Webbook |
| log10ws | -1.78 | | Crippen Method |
| logp | 0.809 | | Crippen Method |
| mcvol | 73.900 | ml/mol | McGowan Method |
| pc | 4782.59 | kPa | Joback Method |
| tb | 321.08 | K | Joback Method |
| tc | 520.62 | K | Joback Method |
| tf | 246.24 | K | Joback Method |
| vc | 0.276 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 106.95 | J/mol×K | 321.08 | Joback Method |
| cpg | 113.60 | J/mol×K | 354.34 | Joback Method |
| cpg | 119.75 | J/mol×K | 387.59 | Joback Method |
| cpg | 125.44 | J/mol×K | 420.85 | Joback Method |
| cpg | 130.70 | J/mol×K | 454.11 | Joback Method |
| cpg | 135.55 | J/mol×K | 487.36 | Joback Method |
| cpg | 140.03 | J/mol×K | 520.62 | Joback Method |

# Sources

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|---|---|
| **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=C6929948&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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