# 4-octyne, 2,7-dimethyl

**Inchi:** InChI=1S/C10H18/c1-9(2)7-5-6-8-10(3)4/h9-10H,7-8H2,1-4H3
**InchiKey:** KCLRHUYFDJVIFV-UHFFFAOYSA-N
**Formula:** C10H18
**SMILES:** CC(C)CC#CCC(C)C
**Mol. weight [g/mol]:** 138.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 231.24 | kJ/mol | Joback Method |
| hf | 12.01 | kJ/mol | Joback Method |
| hfus | 17.73 | kJ/mol | Joback Method |
| hvap | 39.23 | kJ/mol | Joback Method |
| log10ws | -3.32 | | Crippen Method |
| logp | 3.082 | | Crippen Method |
| mcvol | 143.160 | ml/mol | McGowan Method |
| pc | 2495.01 | kPa | Joback Method |
| rinpol | 930.00 | | NIST Webbook |
| tb | 436.32 | K | Joback Method |
| tc | 629.38 | K | Joback Method |
| tf | 278.56 | K | Joback Method |
| vc | 0.545 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 288.39 | J/mol×K | 436.32 | Joback Method |
| cpg | 303.69 | J/mol×K | 468.50 | Joback Method |
| cpg | 318.34 | J/mol×K | 500.67 | Joback Method |
| cpg | 332.36 | J/mol×K | 532.85 | Joback Method |
| cpg | 345.76 | J/mol×K | 565.03 | Joback Method |
| cpg | 358.56 | J/mol×K | 597.20 | Joback Method |
| cpg | 370.78 | J/mol×K | 629.38 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R66700&Units=SI |
| **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

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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 |
| **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 |