# 3-Octyne, 2,2-dimethyl-

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|---|---|
| **Other names:** | 2,2-Dimethyl-3-octyne |
| **Inchi:** | InChI=1S/C10H18/c1-5-6-7-8-9-10(2,3)4/h5-7H2,1-4H3 |
| **InchiKey:** | XBLMXBDWMYMTLK-UHFFFAOYSA-N |
| **Formula:** | C10H18 |
| **SMILES:** | CCCCC#CC(C)(C)C |
| **Mol. weight [g/mol]:** | 138.25 |
| **CAS:** | 19482-57-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 238.96 | kJ/mol | Joback Method |
| hf | 13.82 | kJ/mol | Joback Method |
| hfus | 17.36 | kJ/mol | Joback Method |
| hvap | 38.71 | kJ/mol | Joback Method |
| log10ws | -3.56 | | Crippen Method |
| logp | 3.226 | | Crippen Method |
| mcvol | 143.160 | ml/mol | McGowan Method |
| pc | 2502.50 | kPa | Joback Method |
| tb | 433.97 | K | Joback Method |
| tc | 630.64 | K | Joback Method |
| tf | 310.98 | K | Joback Method |
| vc | 0.546 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 290.42 | J/mol×K | 433.97 | Joback Method |
| cpg | 306.36 | J/mol×K | 466.75 | Joback Method |
| cpg | 321.48 | J/mol×K | 499.53 | Joback Method |
| cpg | 335.83 | J/mol×K | 532.31 | Joback Method |
| cpg | 349.43 | J/mol×K | 565.08 | Joback Method |
| cpg | 362.32 | J/mol×K | 597.86 | Joback Method |
| cpg | 374.53 | J/mol×K | 630.64 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.44054e+01 |
| Coeff. B | -3.76269e+03 |
| Coeff. C | -6.24000e+01 |
| Temperature range (K), min. | 328.92 |
| Temperature range (K), max. | 476.16 |

# 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=C19482576&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 |

# 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 |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |

| | |
|---|---|
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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