# 4-Hepten-3-one, 5-methyl-

**Other names:** 5-Methyl-4-hepten-3-one
**Inchi:** InChI=1S/C8H14O/c1-4-7(3)6-8(9)5-2/h6H,4-5H2,1-3H3/b7-6+
**InchiKey:** XJEHTASYOBAEDB-VOTSOKGWSA-N
**Formula:** C8H14O
**SMILES:** CCC(=O)C=C(C)CC
**Mol. weight [g/mol]:** 126.20
**CAS:** 1447-26-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -40.77 | kJ/mol | Joback Method |
| hf | -213.60 | kJ/mol | Joback Method |
| hfus | 16.97 | kJ/mol | Joback Method |
| hvap | 40.19 | kJ/mol | Joback Method |
| log10ws | -2.30 | | Crippen Method |
| logp | 2.322 | | Crippen Method |
| mcvol | 120.850 | ml/mol | McGowan Method |
| pc | 2871.95 | kPa | Joback Method |
| rinpol | 1007.00 | | NIST Webbook |
| ripol | 1660.00 | | NIST Webbook |
| tb | 438.00 ± 3.00 | K | NIST Webbook |
| tb | 439.70 | K | NIST Webbook |
| tc | 627.87 | K | Joback Method |
| tf | 210.81 | K | Joback Method |
| vc | 0.470 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 239.66 | J/mol×K | 440.35 | Joback Method |
| cpg | 252.05 | J/mol×K | 471.60 | Joback Method |
| cpg | 263.86 | J/mol×K | 502.86 | Joback Method |
| cpg | 275.09 | J/mol×K | 534.11 | Joback Method |
| cpg | 285.78 | J/mol×K | 565.36 | Joback Method |

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|---|---|---|---|---|
| cpg | 295.94 | J/mol×K | 596.61 | Joback Method |
| cpg | 305.60 | J/mol×K | 627.87 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 339.20 | K | 2.40 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.47129e+01 |
| Coeff. B | -3.79887e+03 |
| Coeff. C | -6.33730e+01 |
| Temperature range (K), min. | 326.72 |
| Temperature range (K), max. | 467.45 |

# Sources

**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=C1447263&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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | 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 |