# 4-PENTEN-2-ONE, 4-METHYL-

| | |
|---|---|
| **Other names:** | 2-Methyl-1-penten-4-one |
| | 2-Methylene-4-pentanal |
| | 4-Methyl-4-penten-2-one |
| | CH3C(O)CH2C(CH3)=CH2 |
| | Isomesityl oxide |
| | Isopropenyl acetone |
| **Inchi:** | InChI=1S/C6H10O/c1-5(2)4-6(3)7/h1,4H2,2-3H3 |
| **InchiKey:** | VADUDTKCGJKNDY-UHFFFAOYSA-N |
| **Formula:** | C6H10O |
| **SMILES:** | C=C(C)CC(C)=O |
| **Mol. weight [g/mol]:** | 98.14 |
| **CAS:** | 3744-02-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3382 | | Cheméo Relay (1.0) |
| gf | -49.99 | kJ/mol | Joback Method |
| hf | -174.79 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 10.30 | kJ/mol | Joback Method |
| hvap | 41.90 | kJ/mol | NIST Webbook |
| ie | 9.01 | eV | Cheméo Relay (1.0) |
| log10ws | -0.83 | | Cheméo Relay (1.0) |
| logp | 1.542 | | Crippen Method |
| mcvol | 92.670 | ml/mol | McGowan Method |
| pc | 3526.27 | kPa | Joback Method |
| rinpol | 790.00 | | NIST Webbook |
| ripol | 1110.00 | | NIST Webbook |
| tb | 390.91 | K | Cheméo Relay (1.0) |
| tc | 581.65 | K | Cheméo Relay (1.0) |
| tf | 200.55 ± 0.20 | K | NIST Webbook |
| vc | 0.331 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 163.39 | J/mol×K | 387.11 | Joback Method |
| cpg | 172.98 | J/mol×K | 417.94 | Joback Method |
| cpg | 182.16 | J/mol×K | 448.78 | Joback Method |
| cpg | 190.92 | J/mol×K | 479.61 | Joback Method |
| cpg | 199.29 | J/mol×K | 510.45 | Joback Method |
| cpg | 207.28 | J/mol×K | 541.28 | Joback Method |
| cpg | 214.90 | J/mol×K | 572.11 | Joback Method |
| hvapt | 36.90 | kJ/mol | 425.00 | NIST Webbook |
| hvapt | 41.10 | kJ/mol | 352.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.34033e+01 |
| Coeff. B | -3.13505e+03 |
| Coeff. C | -5.49620e+01 |
| Temperature range (K), min. | 293.99 |
| Temperature range (K), max. | 442.40 |

# Sources

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3744023&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |