# 2-Pentenal

**Other names:** Pent-2-enal
**Inchi:** InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3
**InchiKey:** DTCCTIQRPGSLPT-UHFFFAOYSA-N
**Formula:** C5H8O
**SMILES:** CCC=CC=O
**Mol. weight [g/mol]:** 84.12
**CAS:** 764-39-6

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -28.08 | kJ/mol | Joback Method |
| hf | -114.89 | kJ/mol | Joback Method |
| hfus | 11.20 | kJ/mol | Joback Method |
| hvap | 33.40 | kJ/mol | Joback Method |
| ie | 9.70 | eV | NIST Webbook |
| log10ws | -1.05 | | Crippen Method |
| logp | 1.151 | | Crippen Method |
| mcvol | 78.580 | ml/mol | McGowan Method |
| pc | 4046.64 | kPa | Joback Method |
| rinpol | 676.77 | | NIST Webbook |
| rinpol | 674.28 | | NIST Webbook |
| rinpol | 674.91 | | NIST Webbook |
| rinpol | 675.32 | | NIST Webbook |
| rinpol | 675.72 | | NIST Webbook |
| rinpol | 675.36 | | NIST Webbook |
| rinpol | 677.72 | | NIST Webbook |
| rinpol | 678.55 | | NIST Webbook |
| rinpol | 678.68 | | NIST Webbook |
| rinpol | 680.44 | | NIST Webbook |
| rinpol | 682.23 | | NIST Webbook |
| rinpol | 686.31 | | NIST Webbook |
| rinpol | 700.44 | | NIST Webbook |
| rinpol | 698.24 | | NIST Webbook |
| rinpol | 699.75 | | NIST Webbook |
| rinpol | 700.64 | | NIST Webbook |
| rinpol | 701.70 | | NIST Webbook |
| rinpol | 702.48 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 704.71 | | NIST Webbook |
| rinpol | 705.68 | | NIST Webbook |
| rinpol | 707.08 | | NIST Webbook |
| rinpol | 700.64 | | NIST Webbook |
| rinpol | 713.43 | | NIST Webbook |
| rinpol | 717.73 | | NIST Webbook |
| rinpol | 735.00 | | NIST Webbook |
| rinpol | 721.00 | | NIST Webbook |
| rinpol | 721.00 | | NIST Webbook |
| rinpol | 726.00 | | NIST Webbook |
| rinpol | 738.00 | | NIST Webbook |
| rinpol | 718.00 | | NIST Webbook |
| rinpol | 719.00 | | NIST Webbook |
| rinpol | 725.00 | | NIST Webbook |
| rinpol | 735.00 | | NIST Webbook |
| rinpol | 723.00 | | NIST Webbook |
| rinpol | 735.00 | | NIST Webbook |
| rinpol | 675.36 | | NIST Webbook |
| rinpol | 676.77 | | NIST Webbook |
| rinpol | 725.00 | | NIST Webbook |
| rinpol | 710.42 | | NIST Webbook |
| rinpol | 707.08 | | NIST Webbook |
| rinpol | 682.23 | | NIST Webbook |
| ripol | 1043.00 | | NIST Webbook |
| ripol | 1064.46 | | NIST Webbook |
| ripol | 1073.00 | | NIST Webbook |
| ripol | 1073.00 | | NIST Webbook |
| ripol | 1087.98 | | NIST Webbook |
| ripol | 1078.94 | | NIST Webbook |
| ripol | 1043.68 | | NIST Webbook |
| tb | 397.00 ± 3.00 | K | NIST Webbook |
| tc | 548.86 | K | Joback Method |
| tf | 183.03 | K | Joback Method |
| vc | 0.312 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 130.02 | J/mol×K | 366.62 | Joback Method |
| cpg | 166.65 | J/mol×K | 518.49 | Joback Method |
| cpg | 160.05 | J/mol×K | 488.11 | Joback Method |

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|---|---|---|---|---|
| cpg | 153.10 | J/mol×K | 457.74 | Joback Method |
| cpg | 145.79 | J/mol×K | 427.37 | Joback Method |
| cpg | 138.10 | J/mol×K | 396.99 | Joback Method |
| cpg | 172.92 | J/mol×K | 548.86 | Joback Method |
| dvisc | 0.0002502 | Pa×s | 366.62 | Joback Method |
| dvisc | 0.0003168 | Pa×s | 336.02 | Joback Method |
| dvisc | 0.0004205 | Pa×s | 305.42 | Joback Method |
| dvisc | 0.0005946 | Pa×s | 274.82 | Joback Method |
| dvisc | 0.0009169 | Pa×s | 244.23 | Joback Method |
| dvisc | 0.0016007 | Pa×s | 213.63 | Joback Method |
| dvisc | 0.0033669 | Pa×s | 183.03 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.49143e+01 |
| Coeff. B | -3.55666e+03 |
| Coeff. C | -5.15580e+01 |
| Temperature range (K), min. | 294.72 |
| Temperature range (K), max. | 421.93 |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C764396&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |

| | |
|---|---|
| **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 |
| **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 |

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