# Pentanal, 3-methyl-

| | |
|---|---|
| **Other names:** | 3-Ethylbutanal |
| | 3-Methylpentanal |
| | 3-methylvaleraldehyde |
| | C2H5CH(CH3)CH2CHO |
| | Valeraldehyde, 3-methyl- |
| **Inchi:** | InChI=1S/C6H12O/c1-3-6(2)4-5-7/h5-6H,3-4H2,1-2H3 |
| **InchiKey:** | YJWJGLQYQJGEEP-UHFFFAOYSA-N |
| **Formula:** | C6H12O |
| **SMILES:** | CCC(C)CC=O |
| **Mol. weight [g/mol]:** | 100.16 |
| **CAS:** | 15877-57-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -102.32 | kJ/mol | Joback Method |
| hf | -258.03 | kJ/mol | Joback Method |
| hfus | 10.06 | kJ/mol | Joback Method |
| hvap | 35.28 | kJ/mol | Joback Method |
| ie | 9.90 | eV | NIST Webbook |
| ie | 9.68 | eV | NIST Webbook |
| log10ws | -1.37 | | Crippen Method |
| logp | 1.621 | | Crippen Method |
| mcvol | 96.970 | ml/mol | McGowan Method |
| pc | 3411.87 | kPa | Joback Method |
| rinpol | 719.00 | | NIST Webbook |
| rinpol | 719.00 | | NIST Webbook |
| ripol | 1037.00 | | NIST Webbook |
| ripol | 1026.00 | | NIST Webbook |
| tb | 395.15 ± 2.00 | K | NIST Webbook |
| tc | 561.39 | K | Joback Method |
| tf | 184.38 | K | Joback Method |
| vc | 0.383 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 179.50 | J/mol×K | 384.90 | Joback Method |
| cpg | 189.59 | J/mol×K | 414.32 | Joback Method |
| cpg | 199.28 | J/mol×K | 443.73 | Joback Method |
| cpg | 208.60 | J/mol×K | 473.15 | Joback Method |
| cpg | 217.54 | J/mol×K | 502.56 | Joback Method |
| cpg | 226.11 | J/mol×K | 531.98 | Joback Method |
| cpg | 234.32 | J/mol×K | 561.39 | Joback Method |
| dvisc | 0.0070161 | Pa×s | 184.38 | Joback Method |
| dvisc | 0.0027952 | Pa×s | 217.80 | Joback Method |
| dvisc | 0.0014226 | Pa×s | 251.22 | Joback Method |
| dvisc | 0.0008484 | Pa×s | 284.64 | Joback Method |
| dvisc | 0.0005641 | Pa×s | 318.06 | Joback Method |
| dvisc | 0.0004053 | Pa×s | 351.48 | Joback Method |
| dvisc | 0.0003084 | Pa×s | 384.90 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.63803e+01 |
| Coeff. B | -3.99325e+03 |
| Coeff. C | -5.12800e+01 |
| Temperature range (K), min. | 299.42 |
| Temperature range (K), max. | 412.04 |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C15877573&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

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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 |