# Hexanal, 2-ethyl-

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|---|---|
| **Other names:** | 2-Ethylcaproaldehyde |
| | 2-Ethylhexaldehyde |
| | 2-Ethylhexan-1-al |
| | 2-Ethylhexanal |
| | 2-Ethylhexylaldehyde |
| | 3-Formylheptane |
| | Butylethylacetaldehyde |
| | Ethylbutylacetaldehyde |
| | NSC 42871 |
| | «alpha»-Ethylcaproaldehyde |
| | «alpha»-Ethylhexanal |
| | Â«alphaÂ»-Ethylcaproaldehyde |
| | Â«alphaÂ»-Ethylhexanal |
| **Inchi:** | InChI=1S/C8H16O/c1-3-5-6-8(4-2)7-9/h7-8H,3-6H2,1-2H3 |
| **InchiKey:** | LGYNIFWIKSEESD-UHFFFAOYSA-N |
| **Formula:** | C8H16O |
| **SMILES:** | CCCCC(C=O)CC |
| **Mol. weight [g/mol]:** | 128.21 |
| **CAS:** | 123-05-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -5086.20 ± 0.75 | kJ/mol | NIST Webbook |
| gf | -85.48 | kJ/mol | Joback Method |
| hf | -299.31 | kJ/mol | Joback Method |
| hfl | -348.60 ± 0.75 | kJ/mol | NIST Webbook |
| hfus | 15.24 | kJ/mol | Joback Method |
| hvap | 39.73 | kJ/mol | Joback Method |
| log10ws | -2.13 | | Estimated Solubility Method |
| log10ws | -2.13 | | Aqueous Solubility Prediction Method |
| logp | 2.402 | | Crippen Method |
| mcvol | 125.150 | ml/mol | McGowan Method |
| pc | 2758.46 | kPa | Joback Method |
| rinpol | 938.00 | | NIST Webbook |
| rinpol | 959.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 933.00 | | NIST Webbook |
| rinpol | 935.00 | | NIST Webbook |
| rinpol | 959.00 | | NIST Webbook |
| rinpol | 933.00 | | NIST Webbook |
| rinpol | 933.00 | | NIST Webbook |
| rinpol | 941.00 | | NIST Webbook |
| rinpol | 959.00 | | NIST Webbook |
| rinpol | 933.00 | | NIST Webbook |
| rinpol | 963.00 | | NIST Webbook |
| rinpol | 954.50 | | NIST Webbook |
| rinpol | 956.00 | | NIST Webbook |
| rinpol | 941.00 | | NIST Webbook |
| rinpol | 926.00 | | NIST Webbook |
| rinpol | 933.00 | | NIST Webbook |
| rinpol | 940.00 | | NIST Webbook |
| rinpol | 932.00 | | NIST Webbook |
| rinpol | 940.00 | | NIST Webbook |
| ripol | 1216.00 | | NIST Webbook |
| ripol | 1220.60 | | NIST Webbook |
| ripol | 1216.00 | | NIST Webbook |
| ripol | 1220.60 | | NIST Webbook |
| ripol | 1197.80 | | NIST Webbook |
| ripol | 1205.90 | | NIST Webbook |
| ripol | 1213.10 | | NIST Webbook |
| ripol | 1198.00 | | NIST Webbook |
| tb | 437.15 | K | NIST Webbook |
| tb | 434.65 ± 3.00 | K | NIST Webbook |
| tb | 433.15 ± 2.00 | K | NIST Webbook |
| tc | 605.22 | K | Joback Method |
| tf | 206.92 | K | Joback Method |
| vc | 0.494 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 256.75 | J/mol×K | 430.66 | Joback Method |
| cpg | 314.39 | J/mol×K | 576.13 | Joback Method |
| cpg | 303.81 | J/mol×K | 547.04 | Joback Method |
| cpg | 292.77 | J/mol×K | 517.94 | Joback Method |
| cpg | 281.26 | J/mol×K | 488.85 | Joback Method |
| cpg | 269.26 | J/mol×K | 459.75 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 324.51 | J/mol×K | 605.22 | Joback Method |
| dvisc | 0.0003026 | Pa×s | 430.66 | Joback Method |
| dvisc | 0.0004023 | Pa×s | 393.37 | Joback Method |
| dvisc | 0.0005678 | Pa×s | 356.08 | Joback Method |
| dvisc | 0.0008686 | Pa×s | 318.79 | Joback Method |
| dvisc | 0.0014872 | Pa×s | 281.50 | Joback Method |
| dvisc | 0.0030008 | Pa×s | 244.21 | Joback Method |
| dvisc | 0.0077983 | Pa×s | 206.92 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 328.20 | K | 1.70 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.53956e+01 |
| Coeff. B | -4.04583e+03 |
| Coeff. C | -6.17460e+01 |
| Temperature range (K), min. | 329.54 |
| Temperature range (K), max. | 462.95 |

# Sources

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

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**Estimated Solubility Method:** http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C123057&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

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase 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 |