# 3-Hexanol, 2,4-dimethyl-

**Other names:** 2,4-Dimethyl-3-hexanol
2,4-dimethylhexan-3-ol
**Inchi:** InChI=1S/C8H18O/c1-5-7(4)8(9)6(2)3/h6-9H,5H2,1-4H3
**InchiKey:** UCRQJBCLZKHOGX-UHFFFAOYSA-N
**Formula:** C8H18O
**SMILES:** CCC(C)C(O)C(C)C
**Mol. weight [g/mol]:** 130.23
**CAS:** 13432-25-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -127.66 | kJ/mol | Joback Method |
| hf | -376.52 | kJ/mol | Joback Method |
| hfus | 9.99 | kJ/mol | Joback Method |
| hvap | 48.92 | kJ/mol | Joback Method |
| log10ws | -2.06 | | Crippen Method |
| logp | 2.049 | | Crippen Method |
| mcvol | 129.450 | ml/mol | McGowan Method |
| pc | 2859.68 | kPa | Joback Method |
| tb | 433.00 ± 3.00 | K | NIST Webbook |
| tb | 433.65 ± 3.00 | K | NIST Webbook |
| tb | 433.00 ± 3.00 | K | NIST Webbook |
| tb | 430.15 ± 3.00 | K | NIST Webbook |
| tb | 434.20 | K | NIST Webbook |
| tc | 642.89 | K | Joback Method |
| tf | 195.74 | K | Joback Method |
| vc | 0.484 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 290.54 | J/mol×K | 473.30 | Joback Method |
| cpg | 303.02 | J/mol×K | 501.56 | Joback Method |
| cpg | 314.99 | J/mol×K | 529.83 | Joback Method |

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|---|---|---|---|---|
| cpg | 326.48 | J/mol×K | 558.09 | Joback Method |
| cpg | 337.49 | J/mol×K | 586.36 | Joback Method |
| cpg | 348.04 | J/mol×K | 614.62 | Joback Method |
| cpg | 358.15 | J/mol×K | 642.89 | Joback Method |
| dvisc | 0.9006667 | Pa×s | 195.74 | Joback Method |
| dvisc | 0.0532070 | Pa×s | 242.00 | Joback Method |
| dvisc | 0.0077930 | Pa×s | 288.26 | Joback Method |
| dvisc | 0.0019417 | Pa×s | 334.52 | Joback Method |
| dvisc | 0.0006781 | Pa×s | 380.78 | Joback Method |
| dvisc | 0.0002974 | Pa×s | 427.04 | Joback Method |
| dvisc | 0.0001533 | Pa×s | 473.30 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.75443e+01 |
| Coeff. B | -5.84358e+03 |
| Coeff. C | 1.78800e+01 |
| Temperature range (K), min. | 320.75 |
| Temperature range (K), max. | 459.82 |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C13432252&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 |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |