# 3-Pentanol, 2,4-dimethyl-

| | |
|---|---|
| **Other names:** | 2,4-Dimethyl-3-hydroxypentane |
| | 2,4-Dimethyl-3-pentanol |
| | 2,4-dimethylpentan-3-ol |
| | Diisopropylcarbinol |
| | Diisopropylmethanol |
| **Inchi:** | InChI=1S/C7H16O/c1-5(2)7(8)6(3)4/h5-8H,1-4H3 |
| **InchiKey:** | BAYAKMPRFGNNFW-UHFFFAOYSA-N |
| **Formula:** | C7H16O |
| **SMILES:** | CC(C)C(O)C(C)C |
| **Mol. weight [g/mol]:** | 116.20 |
| **CAS:** | 600-36-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -136.08 | kJ/mol | Joback Method |
| hf | -355.88 | kJ/mol | Joback Method |
| hfus | 7.41 | kJ/mol | Joback Method |
| hvap | 46.69 | kJ/mol | Joback Method |
| log10ws | -1.22 | | Aqueous Solubility Prediction Method |
| log10ws | -1.22 | | Estimated Solubility Method |
| logp | 1.659 | | Crippen Method |
| mcvol | 115.360 | ml/mol | McGowan Method |
| pc | 3177.55 | kPa | Joback Method |
| rinpol | 821.00 | | NIST Webbook |
| rinpol | 132.11 | | NIST Webbook |
| rinpol | 821.00 | | NIST Webbook |
| rinpol | 828.00 | | NIST Webbook |
| rinpol | 821.00 | | NIST Webbook |
| rinpol | 828.00 | | NIST Webbook |
| rinpol | 838.00 | | NIST Webbook |
| rinpol | 827.00 | | NIST Webbook |
| rinpol | 831.00 | | NIST Webbook |
| rinpol | 132.11 | | NIST Webbook |
| rinpol | 820.00 | | NIST Webbook |
| ripol | 1220.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| ripol | 1187.00 | | NIST Webbook |
| ripol | 1157.00 | | NIST Webbook |
| ripol | 1220.00 | | NIST Webbook |
| ripol | 1157.00 | | NIST Webbook |
| ripol | 1157.00 | | NIST Webbook |
| tb | 412.05 ± 1.00 | K | NIST Webbook |
| tb | 412.15 ± 5.00 | K | NIST Webbook |
| tb | 418.15 ± 5.00 | K | NIST Webbook |
| tb | 410.65 ± 3.00 | K | NIST Webbook |
| tb | 413.15 ± 3.00 | K | NIST Webbook |
| tb | 404.65 ± 3.00 | K | NIST Webbook |
| tb | 411.65 ± 3.00 | K | NIST Webbook |
| tb | 411.75 ± 1.00 | K | NIST Webbook |
| tb | 410.65 ± 1.50 | K | NIST Webbook |
| tb | 409.15 ± 3.00 | K | NIST Webbook |
| tb | 412.15 ± 3.00 | K | NIST Webbook |
| tb | 412.15 ± 3.00 | K | NIST Webbook |
| tb | 408.15 ± 3.00 | K | NIST Webbook |
| tb | 412.65 ± 3.00 | K | NIST Webbook |
| tb | 413.15 ± 3.00 | K | NIST Webbook |
| tb | 411.90 | K | NIST Webbook |
| tb | 409.65 ± 2.00 | K | NIST Webbook |
| tb | 411.80 ± 1.00 | K | NIST Webbook |
| tc | 621.17 | K | Joback Method |
| tf | 260.70 | K | Calorimetric and FTIR study of selected aliphatic heptanols |
| vc | 0.428 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 301.14 | J/mol×K | 592.71 | Joback Method |
| cpg | 270.66 | J/mol×K | 507.34 | Joback Method |
| cpg | 259.63 | J/mol×K | 478.88 | Joback Method |
| cpg | 248.14 | J/mol×K | 450.42 | Joback Method |
| cpg | 281.25 | J/mol×K | 535.79 | Joback Method |
| cpg | 310.46 | J/mol×K | 621.17 | Joback Method |
| cpg | 291.41 | J/mol×K | 564.25 | Joback Method |
| dvisc | 1.4537054 | Pa×s | 184.47 | Joback Method |
| dvisc | 0.0001848 | Pa×s | 450.42 | Joback Method |
| dvisc | 0.0003644 | Pa×s | 406.09 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0008488 | Pa×s | 361.77 | Joback Method |
| dvisc | 0.0025037 | Pa×s | 317.44 | Joback Method |
| dvisc | 0.0104915 | Pa×s | 273.12 | Joback Method |
| dvisc | 0.0765956 | Pa×s | 228.79 | Joback Method |
| hvapt | 53.60 | kJ/mol | 359.50 | NIST Webbook |
| hvapt | 48.80 | kJ/mol | 343.00 | NIST Webbook |
| hvapt | 51.80 | kJ/mol | 328.00 | NIST Webbook |
| hvapt | 45.70 | kJ/mol | 358.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.58493e+01 |
| Coeff. B | -3.89667e+03 |
| Coeff. C | -6.40440e+01 |
| Temperature range (K), min. | 314.44 |
| Temperature range (K), max. | 433.82 |

# Sources

| | |
|---|---|
| **Effect of Isomerism on the Liquid-Liquid Phase Behavior of Mixtures of 1-Alkyl-3-methylimidazolium Bis((trifluoromethyl)sulfonyl)amide Ionic Liquids with Heptanol:** | https://www.doi.org/10.1021/acs.jced.8b01203 |
| **Calorimetric and FTIR study of selected aliphatic heptanols:** | https://www.doi.org/10.1016/j.fluid.2016.04.003 |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **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=C600362&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |