# 1-Pentanol, 2,2,4-trimethyl-

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|---|---|
| **Other names:** | (dl) 2,4,4-trimethyl-1-pentanol |
| | 2,2,4-Trimethyl-1-pentanol |
| | 2,2,4-Trimethylpentanol |
| | 2,2,4-trimethylpentan-1-ol |
| **Inchi:** | InChI=1S/C8H18O/c1-7(2)5-8(3,4)6-9/h7,9H,5-6H2,1-4H3 |
| **InchiKey:** | CWPPDTVYIJETDF-UHFFFAOYSA-N |
| **Formula:** | C8H18O |
| **SMILES:** | CC(C)CC(C)(C)CO |
| **Mol. weight [g/mol]:** | 130.23 |
| **CAS:** | 123-44-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -119.94 | kJ/mol | Joback Method |
| hf | -374.71 | kJ/mol | Joback Method |
| hfus | 9.63 | kJ/mol | Joback Method |
| hvap | 48.40 | kJ/mol | Joback Method |
| log10ws | -1.95 | | Crippen Method |
| logp | 2.051 | | Crippen Method |
| mcvol | 129.450 | ml/mol | McGowan Method |
| pc | 2868.87 | kPa | Joback Method |
| ripol | 1326.00 | | NIST Webbook |
| ripol | 1326.00 | | NIST Webbook |
| ripol | 1326.00 | | NIST Webbook |
| tb | 438.15 ± 3.00 | K | NIST Webbook |
| tb | 439.15 ± 3.00 | K | NIST Webbook |
| tb | 439.40 ± 3.00 | K | NIST Webbook |
| tc | 643.32 | K | Joback Method |
| tf | 228.16 | K | Joback Method |
| vc | 0.485 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 292.99 | J/mol×K | 470.95 | Joback Method |
| cpg | 305.85 | J/mol×K | 499.68 | Joback Method |
| cpg | 318.10 | J/mol×K | 528.41 | Joback Method |
| cpg | 329.77 | J/mol×K | 557.13 | Joback Method |
| cpg | 340.87 | J/mol×K | 585.86 | Joback Method |
| cpg | 351.43 | J/mol×K | 614.59 | Joback Method |
| cpg | 361.48 | J/mol×K | 643.32 | Joback Method |
| dvisc | 0.0001719 | Pa×s | 470.95 | Joback Method |
| dvisc | 0.0230030 | Pa×s | 268.62 | Joback Method |
| dvisc | 0.1736472 | Pa×s | 228.16 | Joback Method |
| dvisc | 0.0016435 | Pa×s | 349.55 | Joback Method |
| dvisc | 0.0006624 | Pa×s | 390.02 | Joback Method |
| dvisc | 0.0003167 | Pa×s | 430.49 | Joback Method |
| dvisc | 0.0051732 | Pa×s | 309.09 | Joback Method |
| hvapt | 60.60 ± 0.10 | kJ/mol | 328.00 | NIST Webbook |
| hvapt | 58.60 ± 0.10 | kJ/mol | 343.00 | NIST Webbook |
| hvapt | 56.50 ± 0.10 | kJ/mol | 358.00 | NIST Webbook |
| hvapt | 54.20 | kJ/mol | 399.00 | NIST Webbook |
| hvapt | 54.70 | kJ/mol | 387.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.60428e+01 |
| Coeff. B | -4.22553e+03 |
| Coeff. C | -6.82830e+01 |
| Temperature range (K), min. | 336.48 |
| Temperature range (K), max. | 462.04 |

# 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=C123444&Units=SI

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |