# 3-Heptanol, 3,5-dimethyl-

**Other names:** 3,5-Dimethyl-3-heptanol
**Inchi:** InChI=1S/C9H20O/c1-5-8(3)7-9(4,10)6-2/h8,10H,5-7H2,1-4H3
**InchiKey:** NOSOEGQGQOMHBF-UHFFFAOYSA-N
**Formula:** C9H20O
**SMILES:** CCC(C)CC(C)(O)CC
**Mol. weight [g/mol]:** 144.25
**CAS:** 19549-74-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -111.52 | kJ/mol | Joback Method |
| hf | -395.35 | kJ/mol | Joback Method |
| hfus | 12.22 | kJ/mol | Joback Method |
| hvap | 50.62 | kJ/mol | Joback Method |
| log10ws | -2.72 | | Crippen Method |
| logp | 2.584 | | Crippen Method |
| mcvol | 143.540 | ml/mol | McGowan Method |
| pc | 2595.13 | kPa | Joback Method |
| tb | 493.83 | K | Joback Method |
| tc | 664.90 | K | Joback Method |
| tf | 239.43 | K | Joback Method |
| vc | 0.541 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 337.46 | J/mol×K | 493.83 | Joback Method |
| cpg | 351.13 | J/mol×K | 522.34 | Joback Method |
| cpg | 364.17 | J/mol×K | 550.85 | Joback Method |
| cpg | 376.59 | J/mol×K | 579.36 | Joback Method |
| cpg | 388.42 | J/mol×K | 607.88 | Joback Method |
| cpg | 399.69 | J/mol×K | 636.39 | Joback Method |
| cpg | 410.41 | J/mol×K | 664.90 | Joback Method |
| dvisc | 0.1242076 | Pa×s | 239.43 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0170986 | Pa×s | 281.83 | Joback Method |
| dvisc | 0.0039538 | Pa×s | 324.23 | Joback Method |
| dvisc | 0.0012828 | Pa×s | 366.63 | Joback Method |
| dvisc | 0.0005256 | Pa×s | 409.03 | Joback Method |
| dvisc | 0.0002546 | Pa×s | 451.43 | Joback Method |
| dvisc | 0.0001397 | Pa×s | 493.83 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.48309e+01 |
| Coeff. B | -4.08303e+03 |
| Coeff. C | -6.62500e+01 |
| Temperature range (K), min. | 347.00 |
| Temperature range (K), max. | 495.17 |

# Sources

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C19549747&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

# 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 |

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