# 3-Ethyl-3-methylheptane

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|---|---|
| **Other names:** | 3-Methyl-3-ethylheptane |
| | Heptane, 3-ethyl-3-methyl- |
| **Inchi:** | InChI=1S/C10H22/c1-5-8-9-10(4,6-2)7-3/h5-9H2,1-4H3 |
| **InchiKey:** | HSOMNBKXPGCNBH-UHFFFAOYSA-N |
| **Formula:** | C10H22 |
| **SMILES:** | CCCCC(C)(CC)CC |
| **Mol. weight [g/mol]:** | 142.28 |
| **CAS:** | 17302-01-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 36.16 | kJ/mol | Joback Method |
| hf | -258.48 | kJ/mol | Joback Method |
| hfus | 14.24 | kJ/mol | Joback Method |
| hvap | 47.70 | kJ/mol | NIST Webbook |
| log10ws | -3.77 | | Crippen Method |
| logp | 4.003 | | Crippen Method |
| mcvol | 151.760 | ml/mol | McGowan Method |
| pc | 2145.33 | kPa | Joback Method |
| rinpol | 940.00 | | NIST Webbook |
| rinpol | 940.00 | | NIST Webbook |
| rinpol | 947.80 | | NIST Webbook |
| rinpol | 952.60 | | NIST Webbook |
| rinpol | 953.00 | | NIST Webbook |
| rinpol | 947.50 | | NIST Webbook |
| rinpol | 953.00 | | NIST Webbook |
| rinpol | 953.00 | | NIST Webbook |
| rinpol | 947.80 | | NIST Webbook |
| tb | 437.05 ± 0.40 | K | NIST Webbook |
| tb | 436.95 ± 0.40 | K | NIST Webbook |
| tc | 597.50 | K | Joback Method |
| tf | 204.88 | K | Joback Method |
| vc | 0.585 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 316.97 | J/mol×K | 424.97 | Joback Method |
| cpg | 333.53 | J/mol×K | 453.73 | Joback Method |
| cpg | 349.34 | J/mol×K | 482.48 | Joback Method |
| cpg | 364.44 | J/mol×K | 511.24 | Joback Method |
| cpg | 378.86 | J/mol×K | 539.99 | Joback Method |
| cpg | 392.61 | J/mol×K | 568.75 | Joback Method |
| cpg | 405.72 | J/mol×K | 597.50 | Joback Method |
| dvisc | 0.0108562 | Pa×s | 204.88 | Joback Method |
| dvisc | 0.0035911 | Pa×s | 241.56 | Joback Method |
| dvisc | 0.0015903 | Pa×s | 278.24 | Joback Method |
| dvisc | 0.0008514 | Pa×s | 314.92 | Joback Method |
| dvisc | 0.0005192 | Pa×s | 351.61 | Joback Method |
| dvisc | 0.0003477 | Pa×s | 388.29 | Joback Method |
| dvisc | 0.0002495 | Pa×s | 424.97 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.42220e+01 |
| Coeff. B | -3.64149e+03 |
| Coeff. C | -5.77840e+01 |
| Temperature range (K), min. | 319.11 |
| Temperature range (K), max. | 466.46 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 9.64865e+01 |
| Coeff. B | -8.85162e+03 |
| Coeff. C | -1.19968e+01 |
| Coeff. D | 6.95511e-06 |
| Temperature range (K), min. | 319.15 |

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|---|---|
| Temperature range (K), max. | 620.00 |

# Sources

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|---|---|
| **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 |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol121.mol |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C17302011&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=121 |

# Legend

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|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |