

3-Hepten-1-ol

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|-----------------------------|--|
| Other names: | 3-Heptenol |
| Inchi: | InChI=1S/C7H14O/c1-2-3-4-5-6-7-8/h4-5,8H,2-3,6-7H2,1H3 |
| InchiKey: | SDZQUCJFTUULJX-UHFFFAOYSA-N |
| Formula: | C7H14O |
| SMILES: | CCCC=CCCO |
| Mol. weight [g/mol]: | 114.19 |
| CAS: | 10606-47-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -48.54 | kJ/mol | Joback Method |
| hf | -222.82 | kJ/mol | Joback Method |
| hfus | 18.18 | kJ/mol | Joback Method |
| hvap | 47.81 | kJ/mol | Joback Method |
| log10ws | -1.87 | | Crippen Method |
| logp | 1.725 | | Crippen Method |
| mcvol | 111.060 | ml/mol | McGowan Method |
| pc | 3280.28 | kPa | Joback Method |
| rinpol | 941.00 | | NIST Webbook |
| rinpol | 932.00 | | NIST Webbook |
| rinpol | 940.00 | | NIST Webbook |
| rinpol | 941.00 | | NIST Webbook |
| rinpol | 941.00 | | NIST Webbook |
| rinpol | 941.00 | | NIST Webbook |
| tb | 455.90 | K | Joback Method |
| tc | 623.65 | K | Joback Method |
| tf | 224.39 | K | Joback Method |
| vc | 0.426 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 231.48 | J/molxK | 455.90 | Joback Method |
| cpg | 278.34 | J/molxK | 595.69 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 269.79 | J/mol×K | 567.74 | Joback Method |
| cpg | 260.84 | J/mol×K | 539.78 | Joback Method |
| cpg | 251.49 | J/mol×K | 511.82 | Joback Method |
| cpg | 241.71 | J/mol×K | 483.86 | Joback Method |
| cpg | 286.52 | J/mol×K | 623.65 | Joback Method |
| dvisc | 0.0001710 | Paxs | 455.90 | Joback Method |
| dvisc | 0.0002936 | Paxs | 417.31 | Joback Method |
| dvisc | 0.0005629 | Paxs | 378.73 | Joback Method |
| dvisc | 0.0012506 | Paxs | 340.14 | Joback Method |
| dvisc | 0.0034085 | Paxs | 301.56 | Joback Method |
| dvisc | 0.0124675 | Paxs | 262.97 | Joback Method |
| dvisc | 0.0712349 | Paxs | 224.39 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.59944e+01 |
| Coeff. B | -4.38019e+03 |
| Coeff. C | -6.68480e+01 |
| Temperature range (K), min. | 345.72 |
| Temperature range (K), max. | 476.87 |

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C10606470&Units=SI>

Legend

cpg: Ideal gas heat capacity

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

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