

3,3-Dimethyl-2-pentanol

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| Inchi: | InChI=1S/C7H16O/c1-5-7(3,4)6(2)8/h6,8H,5H2,1-4H3 |
| InchiKey: | FCUOIGTWJDBTHR-UHFFFAOYSA-N |
| Formula: | C7H16O |
| SMILES: | CCC(C)(C)C(C)O |
| Mol. weight [g/mol]: | 116.20 |
| CAS: | 19781-24-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| gf | -128.36 | kJ/mol | Joback Method |
| hf | -354.07 | kJ/mol | Joback Method |
| hfus | 7.04 | kJ/mol | Joback Method |
| hvap | 46.17 | kJ/mol | Joback Method |
| log10ws | -1.89 | | Crippen Method |
| logp | 1.803 | | Crippen Method |
| mcvol | 115.360 | ml/mol | McGowan Method |
| pc | 3188.33 | kPa | Joback Method |
| tb | 420.65 ± 3.00 | K | NIST Webbook |
| tc | 621.71 | K | Joback Method |
| tf | 216.89 | K | Joback Method |
| vc | 0.429 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 250.49 | J/mol×K | 448.07 | Joback Method |
| cpg | 304.69 | J/mol×K | 592.77 | Joback Method |
| cpg | 294.91 | J/mol×K | 563.83 | Joback Method |
| cpg | 284.62 | J/mol×K | 534.89 | Joback Method |
| cpg | 273.81 | J/mol×K | 505.95 | Joback Method |
| cpg | 262.44 | J/mol×K | 477.01 | Joback Method |
| cpg | 313.99 | J/mol×K | 621.71 | Joback Method |
| dvisc | 0.0002114 | Paxs | 448.07 | Joback Method |
| dvisc | 0.0003942 | Paxs | 409.54 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0008366 | Paxs | 371.01 | Joback Method |
| dvisc | 0.0021138 | Paxs | 332.48 | Joback Method |
| dvisc | 0.0068100 | Paxs | 293.95 | Joback Method |
| dvisc | 0.0312263 | Paxs | 255.42 | Joback Method |
| dvisc | 0.2459675 | Paxs | 216.89 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.71798e+01 |
| Coeff. B | -5.44379e+03 |
| Coeff. C | 1.27230e+01 |
| Temperature range (K), min. | 309.54 |
| Temperature range (K), max. | 445.96 |

Sources

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|---|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781249&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 |
| 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 |
| log10ws: | Log10 of Water solubility in mol/l |

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|---------------|-------------------------------------|
| 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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