

3-Octen-1-ol

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|-----------------------------|--|
| Other names: | 3-Octenol Oct-3-en-1-ol Oct-3-en-1-ol (Isomer 2) |
| Inchi: | InChI=1S/C8H16O/c1-2-3-4-5-6-7-8-9/h5-6,9H,2-4,7-8H2,1H3/b6-5+ |
| InchiKey: | YDXQPTHHAPCTPP-AATRIKPKSA-N |
| Formula: | C8H16O |
| SMILES: | CCCCC=CCCO |
| Mol. weight [g/mol]: | 128.21 |
| CAS: | 18185-81-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -40.12 | kJ/mol | Joback Method |
| hf | -243.46 | kJ/mol | Joback Method |
| hfus | 20.77 | kJ/mol | Joback Method |
| hvap | 50.04 | kJ/mol | Joback Method |
| log10ws | -2.29 | | Crippen Method |
| logp | 2.115 | | Crippen Method |
| mcvol | 125.150 | ml/mol | McGowan Method |
| pc | 2947.28 | kPa | Joback Method |
| ripol | 1444.00 | | NIST Webbook |
| ripol | 1438.00 | | NIST Webbook |
| ripol | 1438.00 | | NIST Webbook |
| ripol | 1444.00 | | NIST Webbook |
| ripol | 1440.00 | | NIST Webbook |
| ripol | 1441.00 | | NIST Webbook |
| tb | 478.78 | K | Joback Method |
| tc | 645.49 | K | Joback Method |
| tf | 235.66 | K | Joback Method |
| vc | 0.482 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

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

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|-------|-----------|---------|--------|---------------|
| cpg | 273.29 | J/molxK | 478.78 | Joback Method |
| cpg | 324.63 | J/molxK | 617.71 | Joback Method |
| cpg | 315.25 | J/molxK | 589.92 | Joback Method |
| cpg | 305.44 | J/molxK | 562.14 | Joback Method |
| cpg | 295.20 | J/molxK | 534.35 | Joback Method |
| cpg | 284.49 | J/molxK | 506.57 | Joback Method |
| cpg | 333.60 | J/molxK | 645.49 | Joback Method |
| dvisc | 0.0001449 | Paxs | 478.78 | Joback Method |
| dvisc | 0.0002469 | Paxs | 438.26 | Joback Method |
| dvisc | 0.0004689 | Paxs | 397.74 | Joback Method |
| dvisc | 0.0010300 | Paxs | 357.22 | Joback Method |
| dvisc | 0.0027674 | Paxs | 316.70 | Joback Method |
| dvisc | 0.0099375 | Paxs | 276.18 | Joback Method |
| dvisc | 0.0553869 | Paxs | 235.66 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.55989e+01 |
| Coeff. B | -4.42976e+03 |
| Coeff. C | -7.24080e+01 |
| Temperature range (K), min. | 361.72 |
| Temperature range (K), max. | 503.01 |

Sources

| | |
|---|---|
| Crippen Method: | 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=C18185814&Units=SI |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

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

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