

1-Octyn-3-ol

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|-----------------------------|--|
| Other names: | 1-Octyne-3-ol oct-1-yne-3-ol |
| Inchi: | InChI=1S/C8H14O/c1-3-5-6-7-8(9)4-2/h2,8-9H,3,5-7H2,1H3 |
| InchiKey: | VUGRNZHKYVHZSN-UHFFFAOYSA-N |
| Formula: | C8H14O |
| SMILES: | C#CC(O)CCCC |
| Mol. weight [g/mol]: | 126.20 |
| CAS: | 818-72-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 100.29 | kJ/mol | Joback Method |
| hf | -74.06 | kJ/mol | Joback Method |
| hfus | 20.02 | kJ/mol | Joback Method |
| hvap | 49.55 | kJ/mol | Joback Method |
| log10ws | -2.34 | | Crippen Method |
| logp | 1.561 | | Crippen Method |
| mvol | 120.850 | ml/mol | McGowan Method |
| pc | 3310.55 | kPa | Joback Method |
| tb | 464.30 | K | Joback Method |
| tc | 637.56 | K | Joback Method |
| tf | 272.71 | K | Joback Method |
| vc | 0.459 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 258.70 | J/molxK | 464.30 | Joback Method |
| cpg | 269.22 | J/molxK | 493.18 | Joback Method |
| cpg | 279.29 | J/molxK | 522.05 | Joback Method |
| cpg | 288.91 | J/molxK | 550.93 | Joback Method |
| cpg | 298.10 | J/molxK | 579.81 | Joback Method |
| cpg | 306.89 | J/molxK | 608.69 | Joback Method |
| cpg | 315.27 | J/molxK | 637.56 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.63973e+01 |
| Coeff. B | -4.75406e+03 |
| Coeff. C | -7.38950e+01 |
| Temperature range (K), min. | 369.15 |
| Temperature range (K), max. | 503.15 |

Sources

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|---|---|
| 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=C818724&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/ci9903071 |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| 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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