

# Heptane, 1-ethoxy-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Ether, ethyl heptyl<br>Ethyl heptyl ether          |
| <b>Inchi:</b>               | InChI=1S/C9H20O/c1-3-5-6-7-8-9-10-4-2/h3-9H2,1-2H3 |
| <b>InchiKey:</b>            | UTBWZYCUAYXAKT-UHFFFAOYSA-N                        |
| <b>Formula:</b>             | C9H20O   |
| <b>SMILES:</b>              | CCCCCCCCOCC  |
| <b>Mol. weight [g/mol]:</b> | 144.25   |
| <b>CAS:</b>                 | 1969-43-3  |

## Physical Properties

| Property code | Value         | Unit                 | Source         |
|---------------|---------------|----------------------|----------------|
| gf            | -80.10        | kJ/mol               | Joback Method  |
| hf            | -361.31       | kJ/mol               | Joback Method  |
| hfus          | 20.25         | kJ/mol               | Joback Method  |
| hvap          | 38.04         | kJ/mol               | Joback Method  |
| log10ws       | -2.68         |                      | Crippen Method |
| logp          | 2.993         |                      | Crippen Method |
| mvol          | 143.540       | ml/mol               | McGowan Method |
| pc            | 2269.73       | kPa                  | Joback Method  |
| tb            | 427.74        | K                    | Joback Method  |
| tc            | 591.08        | K                    | Joback Method  |
| tf            | 204.85 ± 0.40 | K                    | NIST Webbook   |
| vc            | 0.557         | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 298.84 | J/mol×K | 427.74          | Joback Method |
| cpg           | 312.62 | J/mol×K | 454.96          | Joback Method |
| cpg           | 325.97 | J/mol×K | 482.19          | Joback Method |
| cpg           | 338.88 | J/mol×K | 509.41          | Joback Method |
| cpg           | 351.35 | J/mol×K | 536.63          | Joback Method |
| cpg           | 363.40 | J/mol×K | 563.86          | Joback Method |
| cpg           | 375.02 | J/mol×K | 591.08          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0042964 | Paxs | 213.42 | Joback Method |
| dvisc | 0.0018183 | Paxs | 249.14 | Joback Method |
| dvisc | 0.0009547 | Paxs | 284.86 | Joback Method |
| dvisc | 0.0005787 | Paxs | 320.58 | Joback Method |
| dvisc | 0.0003878 | Paxs | 356.30 | Joback Method |
| dvisc | 0.0002795 | Paxs | 392.02 | Joback Method |
| dvisc | 0.0002128 | Paxs | 427.74 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1969433&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1969433&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                   |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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