

# 1-Decanol, 2-ethyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2-Ethyl-1-decanol  |
| <b>Inchi:</b>               | InChI=1S/C12H26O/c1-3-5-6-7-8-9-10-12(4-2)11-13/h12-13H,3-11H2,1-2H3 |
| <b>InchiKey:</b>            | LTHQZRHTXDZWX-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H26O  |
| <b>SMILES:</b>              | CCCCCCCCC(CC)CO  |
| <b>Mol. weight [g/mol]:</b> | 186.33   |
| <b>CAS:</b>                 | 21078-65-9   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -89.10  | kJ/mol               | Joback Method  |
| hf            | -448.52 | kJ/mol               | Joback Method  |
| hfus          | 27.40   | kJ/mol               | Joback Method  |
| hvap          | 58.60   | kJ/mol               | Joback Method  |
| log10ws       | -3.87   |                      | Crippen Method |
| logp          | 3.756   |                      | Crippen Method |
| mcvol         | 185.810 | ml/mol               | McGowan Method |
| pc            | 1940.65 | kPa                  | Joback Method  |
| tb            | 565.70  | K                    | Joback Method  |
| tc            | 725.92  | K                    | Joback Method  |
| tf            | 270.82  | K                    | Joback Method  |
| vc            | 0.721   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 478.70    | J/molxK | 565.70          | Joback Method |
| cpg           | 547.50    | J/molxK | 699.22          | Joback Method |
| cpg           | 534.85    | J/molxK | 672.51          | Joback Method |
| cpg           | 521.66    | J/molxK | 645.81          | Joback Method |
| cpg           | 507.92    | J/molxK | 619.11          | Joback Method |
| cpg           | 493.60    | J/molxK | 592.40          | Joback Method |
| cpg           | 559.62    | J/molxK | 725.92          | Joback Method |
| dvisc         | 0.0000810 | Paxs    | 565.70          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001387 | Paxs | 516.55 | Joback Method |
| dvisc | 0.0002660 | Paxs | 467.41 | Joback Method |
| dvisc | 0.0005944 | Paxs | 418.26 | Joback Method |
| dvisc | 0.0016449 | Paxs | 369.11 | Joback Method |
| dvisc | 0.0062239 | Paxs | 319.97 | Joback Method |
| dvisc | 0.0381702 | Paxs | 270.82 | 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=C21078659&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21078659&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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