

# 2-Butenyl ethyl ether

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C6H12O/c1-3-5-6-7-4-2/h3,5H,4,6H2,1-2H3/b5-3+ |
| <b>InchiKey:</b>            | NDYRMWZHBBMBGD-HWKANZROSA-N                            |
| <b>Formula:</b>             | C6H12O   |
| <b>SMILES:</b>              | CC=CCOCC   |
| <b>Mol. weight [g/mol]:</b> | 100.16   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -25.14  | kJ/mol               | Joback Method  |
| hf            | -182.17 | kJ/mol               | Joback Method  |
| hfus          | 12.69   | kJ/mol               | Joback Method  |
| hvap          | 31.32   | kJ/mol               | Joback Method  |
| log10ws       | -1.27   |                      | Crippen Method |
| logp          | 1.599   |                      | Crippen Method |
| mcvol         | 96.970  | ml/mol               | McGowan Method |
| pc            | 3231.98 | kPa                  | Joback Method  |
| rinsol        | 705.00  |                      | NIST Webbook   |
| tb            | 363.26  | K                    | Joback Method  |
| tc            | 536.57  | K                    | Joback Method  |
| tf            | 174.53  | K                    | Joback Method  |
| vc            | 0.369   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 167.70    | J/molxK | 363.26          | Joback Method |
| cpg           | 177.67    | J/molxK | 392.14          | Joback Method |
| cpg           | 187.29    | J/molxK | 421.03          | Joback Method |
| cpg           | 196.56    | J/molxK | 449.91          | Joback Method |
| cpg           | 205.48    | J/molxK | 478.80          | Joback Method |
| cpg           | 214.08    | J/molxK | 507.68          | Joback Method |
| cpg           | 222.34    | J/molxK | 536.57          | Joback Method |
| dvisc         | 0.0032729 | Paxs    | 174.53          | Joback Method |
| dvisc         | 0.0013962 | Paxs    | 205.99          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0007464 | Paxs | 237.44 | Joback Method |
| dvisc | 0.0004620 | Paxs | 268.89 | Joback Method |
| dvisc | 0.0003162 | Paxs | 300.35 | Joback Method |
| dvisc | 0.0002325 | Paxs | 331.80 | Joback Method |
| dvisc | 0.0001803 | Paxs | 363.26 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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>                                 |
| <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=R510984&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R510984&amp;Units=SI</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>rinpol:</b>  | Non-polar retention indices                     |
| <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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