

# Ether, 3,3-dimethyl-1-butenyl ethyl

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C8H16O/c1-5-9-7-6-8(2,3)4/h6-7H,5H2,1-4H3/b7-6+ |
| <b>InchiKey:</b>            | WSGATPNSJGOYHJ-VOTSOKGWSA-N                              |
| <b>Formula:</b>             | C8H16O   |
| <b>SMILES:</b>              | CCOC=CC(C)(C)C   |
| <b>Mol. weight [g/mol]:</b> | 128.21   |
| <b>CAS:</b>                 | 16969-19-0   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -5.46   | kJ/mol  | Joback Method  |
| hf            | -232.20 | kJ/mol  | Joback Method  |
| hfus          | 10.45   | kJ/mol  | Joback Method  |
| hvap          | 34.47   | kJ/mol  | Joback Method  |
| log10ws       | -2.37   |         | Crippen Method |
| logp          | 2.583   |         | Crippen Method |
| mcvol         | 125.150 | ml/mol  | McGowan Method |
| pc            | 2679.08 | kPa     | Joback Method  |
| tb            | 405.79  | K       | Joback Method  |
| tc            | 589.20  | K       | Joback Method  |
| tf            | 199.49  | K       | Joback Method  |
| vc            | 0.470   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 244.32    | J/molxK | 405.79          | Joback Method |
| cpg           | 307.71    | J/molxK | 558.63          | Joback Method |
| cpg           | 296.28    | J/molxK | 528.06          | Joback Method |
| cpg           | 284.25    | J/molxK | 497.49          | Joback Method |
| cpg           | 271.60    | J/molxK | 466.93          | Joback Method |
| cpg           | 258.30    | J/molxK | 436.36          | Joback Method |
| cpg           | 318.56    | J/molxK | 589.20          | Joback Method |
| dvisc         | 0.0001975 | Paxs    | 405.79          | Joback Method |
| dvisc         | 0.0002720 | Paxs    | 371.41          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003998 | Paxs | 337.02 | Joback Method |
| dvisc | 0.0006415 | Paxs | 302.64 | Joback Method |
| dvisc | 0.0011618 | Paxs | 268.26 | Joback Method |
| dvisc | 0.0025060 | Paxs | 233.87 | Joback Method |
| dvisc | 0.0070452 | Paxs | 199.49 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C16969190&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16969190&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>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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