

# Ethanol, 1-ethoxy-2,2,2-trifluoro-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Fluoral ethyl hemiacetal<br>Trifluoroacetaldehyde ethyl hemiacetal<br>Trifluoroacetaldehyde hemiethylacetal<br>1-Ethoxy-2,2,2-trifluoroethanol |
| <b>Inchi:</b>               | InChI=1S/C4H7F3O2/c1-2-9-3(8)4(5,6)7/h3,8H,2H2,1H3   |
| <b>InchiKey:</b>            | KLXJPQNHFFMLIG-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C4H7F3O2   |
| <b>SMILES:</b>              | CCOC(O)C(F)(F)F  |
| <b>Mol. weight [g/mol]:</b> | 144.09   |
| <b>CAS:</b>                 | 433-27-2   |

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -843.05  | kJ/mol  | Joback Method  |
| hf            | -1012.70 | kJ/mol  | Joback Method  |
| hfus          | 9.69     | kJ/mol  | Joback Method  |
| hvap          | 39.45    | kJ/mol  | Joback Method  |
| log10ws       | -1.12    |         | Crippen Method |
| logp          | 0.904    |         | Crippen Method |
| mcvol         | 84.270   | ml/mol  | McGowan Method |
| pc            | 3740.80  | kPa     | Joback Method  |
| tb            | 399.66   | K       | Joback Method  |
| tc            | 550.89   | K       | Joback Method  |
| tf            | 207.08   | K       | Joback Method  |
| vc            | 0.334    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 181.86 | J/molxK | 399.66          | Joback Method |
| cpg           | 189.02 | J/molxK | 424.86          | Joback Method |
| cpg           | 195.88 | J/molxK | 450.07          | Joback Method |
| cpg           | 202.45 | J/molxK | 475.27          | Joback Method |
| cpg           | 208.74 | J/molxK | 500.48          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 214.75 | J/mol×K | 525.68 | Joback Method |
| cpg | 220.48 | J/mol×K | 550.89 | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 377.70 | K    | 99.30          | NIST Webbook |

## 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=C433272&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C433272&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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