

# Ethane, 2-chloro-1,1-dimethoxy-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Acetaldehyde, chloro-, dimethyl acetal<br>Chloroacetaldehyde, dimethyl acetal<br>2-Chloro-1,1-dimethoxyethane<br>2-Chloroacetaldehyde, dimethyl acetal<br>Chlorodimethyl acetal<br>Dimethyl chloroacetal<br>Dimethyl chloracetal |
| <b>Inchi:</b>               | InChI=1S/C4H9ClO2/c1-6-4(3-5)7-2/h4H,3H2,1-2H3   |
| <b>InchiKey:</b>            | CRZJPEIBPQWDGJ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C4H9ClO2   |
| <b>SMILES:</b>              | COC(CCl)OC   |
| <b>Mol. weight [g/mol]:</b> | 124.57   |
| <b>CAS:</b>                 | 97-97-2  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -241.57 | kJ/mol               | Joback Method  |
| hf            | -411.35 | kJ/mol               | Joback Method  |
| hfus          | 9.17    | kJ/mol               | Joback Method  |
| hvap          | 33.31   | kJ/mol               | Joback Method  |
| log10ws       | -0.43   |                      | Crippen Method |
| logp          | 0.844   |                      | Crippen Method |
| mvol          | 91.200  | ml/mol               | McGowan Method |
| pc            | 3607.21 | kPa                  | Joback Method  |
| tb            | 402.20  | K                    | NIST Webbook   |
| tc            | 551.20  | K                    | Joback Method  |
| tf            | 194.22  | K                    | Joback Method  |
| vc            | 0.339   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 159.44 | J/mol×K | 372.75          | Joback Method |
| cpg           | 194.40 | J/mol×K | 521.46          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 187.71    | J/molxK | 491.71 | Joback Method |
| cpg   | 180.86    | J/molxK | 461.97 | Joback Method |
| cpg   | 173.86    | J/molxK | 432.23 | Joback Method |
| cpg   | 166.72    | J/molxK | 402.49 | Joback Method |
| cpg   | 200.92    | J/molxK | 551.20 | Joback Method |
| dvisc | 0.0002355 | Paxs    | 372.75 | Joback Method |
| dvisc | 0.0003071 | Paxs    | 343.00 | Joback Method |
| dvisc | 0.0004212 | Paxs    | 313.24 | Joback Method |
| dvisc | 0.0006172 | Paxs    | 283.49 | Joback Method |
| dvisc | 0.0009892 | Paxs    | 253.73 | Joback Method |
| dvisc | 0.0017972 | Paxs    | 223.97 | Joback Method |
| dvisc | 0.0039208 | Paxs    | 194.22 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C97972&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C97972&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>                               |
| <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>                   |

## 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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