

# Acetaldehyde, methoxy-

|                      |                                                                                                                           |
|----------------------|---------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Methoxyacetaldehyde<br>Acetaldehyde, 2-methoxy-<br>«alpha»-Methoxyacetaldehyde<br>2-Methoxyacetaldehyde<br>Methoxyethanal |
| Inchi:               | InChI=1S/C3H6O2/c1-5-3-2-4/h2H,3H2,1H3                                                                                    |
| InchiKey:            | YSEFYOVWKJXNCH-UHFFFAOYSA-N                                                                                               |
| Formula:             | C3H6O2                                                                                                                    |
| SMILES:              | COCC=O                                                                                                                    |
| Mol. weight [g/mol]: | 74.08                                                                                                                     |
| CAS:                 | 10312-83-1                                                                                                                |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | -230.14       | kJ/mol  | Joback Method  |
| hf            | -323.05       | kJ/mol  | Joback Method  |
| hfus          | 7.00          | kJ/mol  | Joback Method  |
| hvap          | 31.40         | kJ/mol  | Joback Method  |
| log10ws       | 0.55          |         | Crippen Method |
| logp          | -0.168        |         | Crippen Method |
| mcvol         | 60.570        | ml/mol  | McGowan Method |
| pc            | 4762.81       | kPa     | Joback Method  |
| tb            | 365.50 ± 0.50 | K       | NIST Webbook   |
| tc            | 513.09        | K       | Joback Method  |
| tf            | 187.80        | K       | Joback Method  |
| vc            | 0.238         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 101.20 | J/mol×K | 339.12          | Joback Method |
| cpg           | 125.25 | J/mol×K | 484.09          | Joback Method |
| cpg           | 120.65 | J/mol×K | 455.10          | Joback Method |
| cpg           | 115.94 | J/mol×K | 426.10          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 111.13    | J/mol×K | 397.11 | Joback Method |
| cpg   | 106.21    | J/mol×K | 368.11 | Joback Method |
| cpg   | 129.73    | J/mol×K | 513.09 | Joback Method |
| dvisc | 0.0002646 | Pa×s    | 339.12 | Joback Method |
| dvisc | 0.0003280 | Pa×s    | 313.90 | Joback Method |
| dvisc | 0.0004223 | Pa×s    | 288.68 | Joback Method |
| dvisc | 0.0005706 | Pa×s    | 263.46 | Joback Method |
| dvisc | 0.0008217 | Pa×s    | 238.24 | Joback Method |
| dvisc | 0.0012901 | Pa×s    | 213.02 | Joback Method |
| dvisc | 0.0022862 | Pa×s    | 187.80 | Joback Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C10312831&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10312831&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>                             |
| <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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