

# Acetic acid, dimethoxy-, methyl ester

|                      |                                                                                                                                                                                                                                      |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Glyoxylic acid, methyl ester, 2-(dimethyl acetal)<br>Dimethoxyacetic acid methyl ester<br>Glyoxylic acid methyl ester dimethyl acetal<br>Methyl dimethoxyacetate<br>Methyl glyoxylate,dimethyl acetal<br>Methyl 2,2-dimethoxyacetate |
| Inchi:               | InChI=1S/C5H10O4/c1-7-4(6)5(8-2)9-3/h5H,1-3H3                                                                                                                                                                                        |
| InchiKey:            | NZTCVGHPDWAALP-UHFFFAOYSA-N                                                                                                                                                                                                          |
| Formula:             | C5H10O4                                                                                                                                                                                                                              |
| SMILES:              | COC(=O)C(OC)OC                                                                                                                                                                                                                       |
| Mol. weight [g/mol]: | 134.13                                                                                                                                                                                                                               |
| CAS:                 | 89-91-8                                                                                                                                                                                                                              |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -455.14 | kJ/mol  | Joback Method  |
| hf            | -661.05 | kJ/mol  | Joback Method  |
| hfus          | 10.35   | kJ/mol  | Joback Method  |
| hvap          | 40.31   | kJ/mol  | Joback Method  |
| log10ws       | 0.44    |         | Crippen Method |
| logp          | -0.222  |         | Crippen Method |
| mcvol         | 100.490 | ml/mol  | McGowan Method |
| pc            | 3551.53 | kPa     | Joback Method  |
| ripol         | 1442.00 |         | NIST Webbook   |
| ripol         | 1442.00 |         | NIST Webbook   |
| tb            | 434.49  | K       | Joback Method  |
| tc            | 616.90  | K       | Joback Method  |
| tf            | 247.73  | K       | Joback Method  |
| vc            | 0.369   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 205.23 | J/mol×K | 434.49          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 246.36    | J/mol×K | 586.50 | Joback Method |
| cpg   | 238.50    | J/mol×K | 556.10 | Joback Method |
| cpg   | 230.43    | J/mol×K | 525.69 | Joback Method |
| cpg   | 222.18    | J/mol×K | 495.29 | Joback Method |
| cpg   | 213.77    | J/mol×K | 464.89 | Joback Method |
| cpg   | 254.00    | J/mol×K | 616.90 | Joback Method |
| dvisc | 0.0002062 | Pa×s    | 434.49 | Joback Method |
| dvisc | 0.0002659 | Pa×s    | 403.36 | Joback Method |
| dvisc | 0.0003578 | Pa×s    | 372.24 | Joback Method |
| dvisc | 0.0005083 | Pa×s    | 341.11 | Joback Method |
| dvisc | 0.0007746 | Pa×s    | 309.98 | Joback Method |
| dvisc | 0.0012971 | Pa×s    | 278.86 | Joback Method |
| dvisc | 0.0024722 | Pa×s    | 247.73 | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 340.20 | K    | 2.40           | NIST Webbook |

## Sources

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                   |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C89918&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C89918&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>ripol:</b>   | Polar retention indices             |
| <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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