

# Methoxyacetaldehyde diethyl acetal

|                      |                                                        |
|----------------------|--------------------------------------------------------|
| Other names:         | Ethane, 1,1-diethoxy-2-methoxy-                        |
| Inchi:               | InChI=1S/C7H16O3/c1-4-9-7(6-8-3)10-5-2/h7H,4-6H2,1-3H3 |
| InchiKey:            | PCYADPMXIIFTP-UHFFFAOYSA-N                             |
| Formula:             | C7H16O3                                                |
| SMILES:              | CCOC(COC)OCC                                           |
| Mol. weight [g/mol]: | 148.20                                                 |
| CAS:                 | 4819-75-4                                              |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -309.38 | kJ/mol  | Joback Method  |
| hf            | -589.75 | kJ/mol  | Joback Method  |
| hfus          | 13.93   | kJ/mol  | Joback Method  |
| hvap          | 38.02   | kJ/mol  | Joback Method  |
| log10ws       | -0.62   |         | Crippen Method |
| logp          | 1.032   |         | Crippen Method |
| mcvol         | 127.100 | ml/mol  | McGowan Method |
| pc            | 2676.31 | kPa     | Joback Method  |
| tb            | 419.20  | K       | NIST Webbook   |
| tc            | 595.08  | K       | Joback Method  |
| tf            | 220.34  | K       | Joback Method  |
| vc            | 0.475   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 266.07    | J/mol×K | 426.38          | Joback Method |
| cpg           | 320.76    | J/mol×K | 566.96          | Joback Method |
| cpg           | 310.35    | J/mol×K | 538.85          | Joback Method |
| cpg           | 299.67    | J/mol×K | 510.73          | Joback Method |
| cpg           | 288.72    | J/mol×K | 482.61          | Joback Method |
| cpg           | 277.52    | J/mol×K | 454.50          | Joback Method |
| cpg           | 330.86    | J/mol×K | 595.08          | Joback Method |
| dvisc         | 0.0001655 | Pa×s    | 426.38          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002194 | Pa×s | 392.04 | Joback Method |
| dvisc | 0.0003071 | Pa×s | 357.70 | Joback Method |
| dvisc | 0.0004618 | Pa×s | 323.36 | Joback Method |
| dvisc | 0.0007650 | Pa×s | 289.02 | Joback Method |
| dvisc | 0.0014520 | Pa×s | 254.68 | Joback Method |
| dvisc | 0.0033654 | Pa×s | 220.34 | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <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=C4819754&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4819754&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>                                       |

## 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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