

# 1,3-Dioxole, 4-methyl-

|                      |                                            |
|----------------------|--------------------------------------------|
| Inchi:               | InChI=1S/C4H6O2/c1-4-2-5-3-6-4/h2H,3H2,1H3 |
| InchiKey:            | OHGDYNKEHUBFCC-UHFFFAOYSA-N                |
| Formula:             | C4H6O2                                     |
| SMILES:              | CC1=COCO1                                  |
| Mol. weight [g/mol]: | 86.09                                      |
| CAS:                 | 14738-96-6                                 |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -124.85 | kJ/mol  | Joback Method  |
| hf            | -262.76 | kJ/mol  | Joback Method  |
| hfus          | 15.77   | kJ/mol  | Joback Method  |
| hvap          | 35.04   | kJ/mol  | Joback Method  |
| log10ws       | -0.91   |         | Crippen Method |
| logp          | 0.852   |         | Crippen Method |
| mcvol         | 63.800  | ml/mol  | McGowan Method |
| pc            | 5205.63 | kPa     | Joback Method  |
| tb            | 368.91  | K       | Joback Method  |
| tc            | 573.29  | K       | Joback Method  |
| tf            | 216.40  | K       | Joback Method  |
| vc            | 0.230   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 111.38    | J/mol×K | 368.91          | Joback Method |
| cpg           | 148.43    | J/mol×K | 539.22          | Joback Method |
| cpg           | 141.83    | J/mol×K | 505.16          | Joback Method |
| cpg           | 134.85    | J/mol×K | 471.10          | Joback Method |
| cpg           | 127.45    | J/mol×K | 437.04          | Joback Method |
| cpg           | 119.64    | J/mol×K | 402.97          | Joback Method |
| cpg           | 154.64    | J/mol×K | 573.29          | Joback Method |
| dvisc         | 0.0003953 | Pa×s    | 368.91          | Joback Method |
| dvisc         | 0.0004981 | Pa×s    | 343.49          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0006513 | Pa×s | 318.07 | Joback Method |
| dvisc | 0.0008921 | Pa×s | 292.65 | Joback Method |
| dvisc | 0.0012974 | Pa×s | 267.24 | Joback Method |
| dvisc | 0.0020415 | Pa×s | 241.82 | Joback Method |
| dvisc | 0.0035731 | Pa×s | 216.40 | Joback Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <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=C14738966&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14738966&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>                                     |

## 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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