

# 1,1-Dimethoxycyclopentane

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C7H14O2/c1-8-7(9-2)5-3-4-6-7/h3-6H2,1-2H3 |
| <b>InchiKey:</b>            | AGWFDZMDKNQQHG-UHFFFAOYSA-N                        |
| <b>Formula:</b>             | C7H14O2  |
| <b>SMILES:</b>              | COC1(OC)CCCC1                                      |
| <b>Mol. weight [g/mol]:</b> | 130.18   |
| <b>CAS:</b>                 | 931-94-2   |

## Physical Properties

| Property code | Value          | Unit                 | Source         |
|---------------|----------------|----------------------|----------------|
| gf            | -170.88        | kJ/mol               | Joback Method  |
| hf            | -397.00 ± 2.00 | kJ/mol               | NIST Webbook   |
| hfl           | -444.00 ± 1.00 | kJ/mol               | NIST Webbook   |
| hfus          | 3.90           | kJ/mol               | Joback Method  |
| hvap          | 44.50 ± 0.30   | kJ/mol               | NIST Webbook   |
| hvap          | 46.07          | kJ/mol               | NIST Webbook   |
| log10ws       | -1.43          |                      | Crippen Method |
| logp          | 1.550          |                      | Crippen Method |
| mcvol         | 110.370        | ml/mol               | McGowan Method |
| pc            | 3464.28        | kPa                  | Joback Method  |
| tb            | 419.92         | K                    | Joback Method  |
| tc            | 622.05         | K                    | Joback Method  |
| tf            | 247.91         | K                    | Joback Method  |
| vc            | 0.403          | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 291.33 | J/mol×K | 588.36          | Joback Method |
| cpg           | 224.74 | J/mol×K | 419.92          | Joback Method |
| cpg           | 239.67 | J/mol×K | 453.61          | Joback Method |
| cpg           | 253.73 | J/mol×K | 487.30          | Joback Method |
| cpg           | 266.98 | J/mol×K | 520.99          | Joback Method |
| cpg           | 279.49 | J/mol×K | 554.68          | Joback Method |
| cpg           | 302.56 | J/mol×K | 622.05          | 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=C931942&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C931942&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>cp<sub>g</sub>:</b>     | Ideal gas heat capacity                                   |
| <b>g<sub>f</sub>:</b>      | Standard Gibbs free energy of formation                   |
| <b>h<sub>f</sub>:</b>      | Enthalpy of formation at standard conditions              |
| <b>h<sub>l</sub>:</b>      | Liquid phase enthalpy of formation at standard conditions |
| <b>h<sub>fus</sub>:</b>    | Enthalpy of fusion at standard conditions                 |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions           |
| <b>h<sub>vapt</sub>:</b>   | Enthalpy of vaporization at a given temperature           |
| <b>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l            |
| <b>log<sub>p</sub>:</b>    | Octanol/Water partition coefficient                       |
| <b>mc<sub>vol</sub>:</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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