

# cis-5-Hydroxy-2-methyl-1,3-dioxane

|                      |                                                            |
|----------------------|------------------------------------------------------------|
| Inchi:               | InChI=1S/C5H10O3/c1-4-7-2-5(6)3-8-4/h4-6H,2-3H2,1H3/t4-,5+ |
| InchiKey:            | RLVMGTURHNLOJX-SYDPRGILSA-N                                |
| Formula:             | C5H10O3                                                    |
| SMILES:              | CC1OCC(O)CO1                                               |
| Mol. weight [g/mol]: | 118.13                                                     |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -301.10 | kJ/mol  | Joback Method  |
| hf            | -528.78 | kJ/mol  | Joback Method  |
| hfus          | 21.66   | kJ/mol  | Joback Method  |
| hvap          | 52.54   | kJ/mol  | Joback Method  |
| log10ws       | 0.03    |         | Crippen Method |
| logp          | -0.260  |         | Crippen Method |
| mcvol         | 88.060  | ml/mol  | McGowan Method |
| pc            | 4743.15 | kPa     | Joback Method  |
| ripol         | 1494.00 |         | NIST Webbook   |
| ripol         | 1494.00 |         | NIST Webbook   |
| tb            | 474.76  | K       | Joback Method  |
| tc            | 670.84  | K       | Joback Method  |
| tf            | 263.21  | K       | Joback Method  |
| vc            | 0.308   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 204.68    | J/mol×K | 474.76          | Joback Method |
| cpg           | 256.23    | J/mol×K | 638.16          | Joback Method |
| cpg           | 246.94    | J/mol×K | 605.48          | Joback Method |
| cpg           | 237.14    | J/mol×K | 572.80          | Joback Method |
| cpg           | 226.84    | J/mol×K | 540.12          | Joback Method |
| cpg           | 216.02    | J/mol×K | 507.44          | Joback Method |
| cpg           | 265.02    | J/mol×K | 670.84          | Joback Method |
| dvisc         | 0.0002631 | Pa×s    | 474.76          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0004246 | Pa×s | 439.50 | Joback Method |
| dvisc | 0.0007446 | Pa×s | 404.24 | Joback Method |
| dvisc | 0.0014541 | Pa×s | 368.99 | Joback Method |
| dvisc | 0.0032707 | Pa×s | 333.73 | Joback Method |
| dvisc | 0.0089098 | Pa×s | 298.47 | Joback Method |
| dvisc | 0.0317470 | Pa×s | 263.21 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=R572180&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R572180&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>                         |

## 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>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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