

# Cyclopentanol,2-methoxy-,cis-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C6H12O2/c1-8-6-4-2-3-5(6)7/h5-7H,2-4H2,1H3/t5-,6+/m0/s1 |
| <b>InchiKey:</b>            | YVXLDOASGKIXII-NTSWFWBYSA-N                                      |
| <b>Formula:</b>             | C6H12O2  |
| <b>SMILES:</b>              | COC1CCCC1O   |
| <b>Mol. weight [g/mol]:</b> | 116.16   |
| <b>CAS:</b>                 | 13051-91-7   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -213.34 | kJ/mol  | Joback Method  |
| hf            | -411.48 | kJ/mol  | Joback Method  |
| hfus          | 11.58   | kJ/mol  | Joback Method  |
| hvap          | 47.99   | kJ/mol  | Joback Method  |
| ie            | 9.80    | eV      | NIST Webbook   |
| log10ws       | -0.80   |         | Crippen Method |
| logp          | 0.546   |         | Crippen Method |
| mcvol         | 96.280  | ml/mol  | McGowan Method |
| pc            | 4046.64 | kPa     | Joback Method  |
| tb            | 461.89  | K       | Joback Method  |
| tc            | 648.35  | K       | Joback Method  |
| tf            | 247.09  | K       | Joback Method  |
| vc            | 0.348   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 213.71    | J/molxK | 461.89          | Joback Method |
| cpg           | 269.01    | J/molxK | 617.27          | Joback Method |
| cpg           | 258.91    | J/molxK | 586.19          | Joback Method |
| cpg           | 248.34    | J/molxK | 555.12          | Joback Method |
| cpg           | 237.29    | J/molxK | 524.04          | Joback Method |
| cpg           | 225.75    | J/molxK | 492.97          | Joback Method |
| cpg           | 278.63    | J/molxK | 648.35          | Joback Method |
| dvisc         | 0.0002369 | Paxs    | 461.89          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003653 | Paxs | 426.09 | Joback Method |
| dvisc | 0.0006099 | Paxs | 390.29 | Joback Method |
| dvisc | 0.0011291 | Paxs | 354.49 | Joback Method |
| dvisc | 0.0024006 | Paxs | 318.69 | Joback Method |
| dvisc | 0.0061775 | Paxs | 282.89 | Joback Method |
| dvisc | 0.0209056 | Paxs | 247.09 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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.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=C13051917&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13051917&amp;Units=SI</a> |

## Legend

|                            |   |
|----------------------------|---|
| <b>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>                 | Ionization energy                               |
| <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>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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