

# Furan, tetrahydro-2,5-dimethyl-, cis-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2,5-Dimethyltetrahydrofuran, (Z)-<br>cis-2,5-Dimethyltetrahydrofuran<br>cis-Tetrahydro-2,5-Dimethylfuran |
| <b>Inchi:</b>               | InChI=1S/C6H12O/c1-5-3-4-6(2)7-5/h5-6H,3-4H2,1-2H3/t5-,6+  |
| <b>InchiKey:</b>            | OXMIDRBAFOEOQT-OLQVQODUSA-N  |
| <b>Formula:</b>             | C6H12O   |
| <b>SMILES:</b>              | CC1CCC(C)O1  |
| <b>Mol. weight [g/mol]:</b> | 100.16   |
| <b>CAS:</b>                 | 2144-41-4  |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | -57.64        | kJ/mol  | Joback Method  |
| hf            | -259.03       | kJ/mol  | Joback Method  |
| hfus          | 14.28         | kJ/mol  | Joback Method  |
| hvap          | 33.41         | kJ/mol  | Joback Method  |
| log10ws       | -1.54         |         | Crippen Method |
| logp          | 1.574         |         | Crippen Method |
| mcvol         | 90.410        | ml/mol  | McGowan Method |
| pc            | 3646.53       | kPa     | Joback Method  |
| tb            | 364.65 ± 1.00 | K       | NIST Webbook   |
| tc            | 569.86        | K       | Joback Method  |
| tf            | 190.61        | K       | Joback Method  |
| vc            | 0.333         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 165.98 | J/molxK | 374.24          | Joback Method |
| cpg           | 229.04 | J/molxK | 537.25          | Joback Method |
| cpg           | 217.59 | J/molxK | 504.65          | Joback Method |
| cpg           | 205.56 | J/molxK | 472.05          | Joback Method |
| cpg           | 192.97 | J/molxK | 439.45          | Joback Method |
| cpg           | 179.78 | J/molxK | 406.84          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 239.94    | J/molxK | 569.86 | Joback Method |
| dvisc | 0.0003240 | Paxs    | 374.24 | Joback Method |
| dvisc | 0.0003887 | Paxs    | 343.63 | Joback Method |
| dvisc | 0.0004833 | Paxs    | 313.03 | Joback Method |
| dvisc | 0.0006300 | Paxs    | 282.43 | Joback Method |
| dvisc | 0.0008757 | Paxs    | 251.82 | Joback Method |
| dvisc | 0.0013336 | Paxs    | 221.22 | Joback Method |
| dvisc | 0.0023244 | Paxs    | 190.61 | Joback Method |

## Sources

|  |   |
|--|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2144414&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2144414&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>Solubilities of gases in cycloethers. The solubility of 13 nonpolar gases in 2 open chain and 4 furan derivatives. Dependence of 20 D<sub>gas</sub> on temperature and pressure. 40.13 kPa.</b> | <a href="https://www.doi.org/10.1016/j.jct.2018.12.037">https://www.doi.org/10.1016/j.jct.2018.12.037</a>                                   |
| <b>Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:</b>  | <a href="https://www.doi.org/10.1021/acs.jced.6b00576">https://www.doi.org/10.1021/acs.jced.6b00576</a>                                     |
|  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
|  | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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