

# Furan, tetrahydro-2,4-dimethyl-, trans-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 2,4-Dimethyltetrahydrofuran, (E)-                               |
| <b>Inchi:</b>               | InChI=1S/C6H12O/c1-5-3-6(2)7-4-5/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1 |
| <b>InchiKey:</b>            | QMGLMRPHOITLSN-WDSKDSINSA-N                                     |
| <b>Formula:</b>             | C6H12O  |
| <b>SMILES:</b>              | CC1COC(C)C1   |
| <b>Mol. weight [g/mol]:</b> | 100.16  |
| <b>CAS:</b>                 | 39168-02-0  |

## 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       | -1.19   |                      | Crippen Method |
| logp          | 1.431   |                      | Crippen Method |
| mcvol         | 90.410  | ml/mol               | McGowan Method |
| pc            | 3646.53 | kPa                  | Joback Method  |
| tb            | 374.24  | K                    | Joback Method  |
| tc            | 569.86  | K                    | Joback Method  |
| tf            | 190.61  | K                    | Joback Method  |
| vc            | 0.333   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 165.98    | J/molxK | 374.24          | Joback Method |
| cpg           | 179.78    | J/molxK | 406.84          | Joback Method |
| cpg           | 192.97    | J/molxK | 439.45          | Joback Method |
| cpg           | 205.56    | J/molxK | 472.05          | Joback Method |
| cpg           | 217.59    | J/molxK | 504.65          | Joback Method |
| cpg           | 229.04    | J/molxK | 537.25          | Joback Method |
| cpg           | 239.94    | J/molxK | 569.86          | Joback Method |
| dvisc         | 0.0023244 | Paxs    | 190.61          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0013336 | Paxs | 221.22 | Joback Method |
| dvisc | 0.0008757 | Paxs | 251.82 | Joback Method |
| dvisc | 0.0006300 | Paxs | 282.43 | Joback Method |
| dvisc | 0.0004833 | Paxs | 313.03 | Joback Method |
| dvisc | 0.0003887 | Paxs | 343.63 | Joback Method |
| dvisc | 0.0003240 | Paxs | 374.24 | 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=C39168020&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C39168020&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>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>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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