

# 3-Furanol, tetrahydro-

|                      |                                                                                                         |
|----------------------|---------------------------------------------------------------------------------------------------------|
| Other names:         | 3-Hydroxytetrahydrofuran<br>Tetrahydro-3-furanol<br>Tetrahydrofuran, 3-hydroxy-<br>tetrahydrofuran-3-ol |
| Inchi:               | InChI=1S/C4H8O2/c5-4-1-2-6-3-4/h4-5H,1-3H2                                                              |
| InchiKey:            | XDPCNPCKDGQBAN-UHFFFAOYSA-N                                                                             |
| Formula:             | C4H8O2                                                                                                  |
| SMILES:              | OC1CCOC1                                                                                                |
| Mol. weight [g/mol]: | 88.11                                                                                                   |
| CAS:                 | 453-20-3                                                                                                |

## Physical Properties

| Property code | Value   | Unit    | Source                                  |
|---------------|---------|---------|-----------------------------------------|
| gf            | -203.59 | kJ/mol  | Joback Method                           |
| hf            | -349.64 | kJ/mol  | Joback Method                           |
| hfus          | 12.12   | kJ/mol  | Joback Method                           |
| hvap          | 45.94   | kJ/mol  | Joback Method                           |
| ie            | 9.77    | eV      | NIST Webbook                            |
| log10ws       | 1.05    |         | Aqueous Solubility<br>Prediction Method |
| logp          | -0.232  |         | Crippen Method                          |
| mcvol         | 68.100  | ml/mol  | McGowan Method                          |
| pc            | 5577.49 | kPa     | Joback Method                           |
| ripol         | 1619.00 |         | NIST Webbook                            |
| tb            | 454.20  | K       | NIST Webbook                            |
| tc            | 616.61  | K       | Joback Method                           |
| tf            | 233.13  | K       | Joback Method                           |
| vc            | 0.240   | m3/kmol | Joback Method                           |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 138.66 | J/mol×K | 425.33          | Joback Method |
| cpg           | 148.01 | J/mol×K | 457.21          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 156.90    | J/mol×K | 489.09 | Joback Method |
| cpg   | 165.32    | J/mol×K | 520.97 | Joback Method |
| cpg   | 173.31    | J/mol×K | 552.85 | Joback Method |
| cpg   | 180.87    | J/mol×K | 584.73 | Joback Method |
| cpg   | 188.01    | J/mol×K | 616.61 | Joback Method |
| dvisc | 0.0517048 | Pa×s    | 233.13 | Joback Method |
| dvisc | 0.0138328 | Pa×s    | 265.16 | Joback Method |
| dvisc | 0.0049173 | Pa×s    | 297.20 | Joback Method |
| dvisc | 0.0021377 | Pa×s    | 329.23 | Joback Method |
| dvisc | 0.0010773 | Pa×s    | 361.26 | Joback Method |
| dvisc | 0.0006070 | Pa×s    | 393.30 | Joback Method |
| dvisc | 0.0003729 | Pa×s    | 425.33 | Joback Method |

## Sources

|                                              |                                                                                                                                                                                                                         |
|----------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <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>Joback Method:</b>                        | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                                                   |
| <b>Aqueous Solubility Prediction Method:</b> | <a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</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=C453203&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C453203&amp;Units=SI</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>ie:</b>      | Ionization energy                               |
| <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                   |

**vc:** Critical Volume

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