

# 2H-Pyran, 4-chlorotetrahydro-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 4-Chlorotetrahydropyran                     |
| <b>Inchi:</b>               | InChI=1S/C5H9ClO/c6-5-1-3-7-4-2-5/h5H,1-4H2 |
| <b>InchiKey:</b>            | DHRSKOBIDIDMJZ-UHFFFAOYSA-N                 |
| <b>Formula:</b>             | C5H9ClO                                     |
| <b>SMILES:</b>              | C1C1CCOCC1                                  |
| <b>Mol. weight [g/mol]:</b> | 120.58                                      |
| <b>CAS:</b>                 | 1768-64-5                                   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -82.38  | kJ/mol               | Joback Method  |
| hf            | -239.95 | kJ/mol               | Joback Method  |
| hfus          | 12.72   | kJ/mol               | Joback Method  |
| hvap          | 36.05   | kJ/mol               | Joback Method  |
| log10ws       | -1.16   |                      | Crippen Method |
| logp          | 1.404   |                      | Crippen Method |
| mcvol         | 88.560  | ml/mol               | McGowan Method |
| pc            | 4222.04 | kPa                  | Joback Method  |
| tb            | 423.20  | K                    | NIST Webbook   |
| tc            | 613.11  | K                    | Joback Method  |
| tf            | 209.98  | K                    | Joback Method  |
| vc            | 0.319   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 154.01    | J/mol×K | 397.73          | Joback Method |
| cpg           | 166.79    | J/mol×K | 433.63          | Joback Method |
| cpg           | 178.89    | J/mol×K | 469.52          | Joback Method |
| cpg           | 190.34    | J/mol×K | 505.42          | Joback Method |
| cpg           | 201.15    | J/mol×K | 541.32          | Joback Method |
| cpg           | 211.34    | J/mol×K | 577.22          | Joback Method |
| cpg           | 220.92    | J/mol×K | 613.11          | Joback Method |
| dvisc         | 0.0073798 | Paxs    | 209.98          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0032986 | Paxs | 241.27 | Joback Method |
| dvisc | 0.0017739 | Paxs | 272.56 | Joback Method |
| dvisc | 0.0010839 | Paxs | 303.86 | Joback Method |
| dvisc | 0.0007261 | Paxs | 335.15 | Joback Method |
| dvisc | 0.0005209 | Paxs | 366.44 | Joback Method |
| dvisc | 0.0003937 | Paxs | 397.73 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C1768645&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1768645&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>                                   |

## Legend

|                                       |   |
|---------------------------------------|---|
| <b>cp<sub>g</sub>:</b>                | Ideal gas heat capacity                         |
| <b>dvisc:</b>                         | Dynamic viscosity                               |
| <b>g<sub>f</sub>:</b>                 | Standard Gibbs free energy of formation         |
| <b>h<sub>f</sub>:</b>                 | Enthalpy of formation at standard conditions    |
| <b>h<sub>fus</sub>:</b>               | Enthalpy of fusion at standard conditions       |
| <b>h<sub>vap</sub>:</b>               | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>w<sub>s</sub>:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</b>               | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</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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