

# 3-Hydroxy-2-pentanone

|                      |                                                                     |
|----------------------|---------------------------------------------------------------------|
| Other names:         | 3-hydroxypentan-2-one<br>2-pentanon-3-ol<br>2-Pentanone, 3-hydroxy- |
| Inchi:               | InChI=1S/C5H10O2/c1-3-5(7)4(2)6/h5,7H,3H2,1-2H3                     |
| InchiKey:            | HDKKRASBPHFULQ-UHFFFAOYSA-N                                         |
| Formula:             | C5H10O2                                                             |
| SMILES:              | CCC(O)C(C)=O                                                        |
| Mol. weight [g/mol]: | 102.13                                                              |
| CAS:                 | 3142-66-3                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -276.96 | kJ/mol | Joback Method  |
| hf            | -416.62 | kJ/mol | Joback Method  |
| hfus          | 10.87   | kJ/mol | Joback Method  |
| hvap          | 49.76   | kJ/mol | Joback Method  |
| log10ws       | -0.57   |        | Crippen Method |
| logp          | 0.346   |        | Crippen Method |
| mcvol         | 88.750  | ml/mol | McGowan Method |
| pc            | 4244.08 | kPa    | Joback Method  |
| rinpol        | 815.00  |        | NIST Webbook   |
| rinpol        | 768.00  |        | NIST Webbook   |
| rinpol        | 783.00  |        | NIST Webbook   |
| rinpol        | 838.00  |        | NIST Webbook   |
| ripol         | 1355.00 |        | NIST Webbook   |
| ripol         | 1338.00 |        | NIST Webbook   |
| ripol         | 1349.00 |        | NIST Webbook   |
| ripol         | 1368.00 |        | NIST Webbook   |
| ripol         | 1345.00 |        | NIST Webbook   |
| ripol         | 1338.00 |        | NIST Webbook   |
| ripol         | 1330.00 |        | NIST Webbook   |
| ripol         | 1340.00 |        | NIST Webbook   |
| ripol         | 1346.00 |        | NIST Webbook   |
| ripol         | 1327.00 |        | NIST Webbook   |
| ripol         | 1344.00 |        | NIST Webbook   |
| ripol         | 1366.00 |        | NIST Webbook   |
| ripol         | 1338.00 |        | NIST Webbook   |

|    |        |                      |               |
|----|--------|----------------------|---------------|
| tb | 459.41 | K                    | Joback Method |
| tc | 635.76 | K                    | Joback Method |
| tf | 241.86 | K                    | Joback Method |
| vc | 0.335  | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 183.94    | J/mol×K | 459.41          | Joback Method |
| cpg           | 191.99    | J/mol×K | 488.80          | Joback Method |
| cpg           | 199.72    | J/mol×K | 518.19          | Joback Method |
| cpg           | 207.12    | J/mol×K | 547.58          | Joback Method |
| cpg           | 214.20    | J/mol×K | 576.97          | Joback Method |
| cpg           | 220.97    | J/mol×K | 606.37          | Joback Method |
| cpg           | 227.44    | J/mol×K | 635.76          | Joback Method |
| dvisc         | 0.0540168 | Pa×s    | 241.86          | Joback Method |
| dvisc         | 0.0120393 | Pa×s    | 278.12          | Joback Method |
| dvisc         | 0.0037936 | Pa×s    | 314.38          | Joback Method |
| dvisc         | 0.0015179 | Pa×s    | 350.63          | Joback Method |
| dvisc         | 0.0007211 | Pa×s    | 386.89          | Joback Method |
| dvisc         | 0.0003892 | Pa×s    | 423.15          | Joback Method |
| dvisc         | 0.0002315 | Pa×s    | 459.41          | 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=C3142663&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3142663&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>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>rinpol:</b>  | Non-polar retention indices                     |
| <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                   |
| <b>vc:</b>      | Critical Volume                                 |

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