

# Benzaldehyde, 2-hydroxy, 5-ethyl

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C9H10O2/c1-2-7-3-4-9(11)8(5-7)6-10/h3-6,11H,2H2,1H3 |
| <b>InchiKey:</b>            | XSTCLZHMZASDDK-UHFFFAOYSA-N                                  |
| <b>Formula:</b>             | C9H10O2  |
| <b>SMILES:</b>              | CCc1ccc(O)c(C=O)c1   |
| <b>Mol. weight [g/mol]:</b> | 150.17   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -126.46 | kJ/mol  | Joback Method  |
| hf            | -266.92 | kJ/mol  | Joback Method  |
| hfus          | 20.79   | kJ/mol  | Joback Method  |
| hvap          | 58.30   | kJ/mol  | Joback Method  |
| log10ws       | -2.06   |         | Crippen Method |
| logp          | 1.767   |         | Crippen Method |
| mcvol         | 121.350 | ml/mol  | McGowan Method |
| pc            | 4200.18 | kPa     | Joback Method  |
| rinpol        | 1496.00 |         | NIST Webbook   |
| tb            | 566.26  | K       | Joback Method  |
| tc            | 792.70  | K       | Joback Method  |
| tf            | 383.85  | K       | Joback Method  |
| vc            | 0.414   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 282.11    | J/molxK | 566.26          | Joback Method |
| cpg           | 292.99    | J/molxK | 604.00          | Joback Method |
| cpg           | 303.11    | J/molxK | 641.74          | Joback Method |
| cpg           | 312.54    | J/molxK | 679.48          | Joback Method |
| cpg           | 321.36    | J/molxK | 717.22          | Joback Method |
| cpg           | 329.64    | J/molxK | 754.96          | Joback Method |
| cpg           | 337.45    | J/molxK | 792.70          | Joback Method |
| dvisc         | 0.0015230 | Paxs    | 383.85          | Joback Method |
| dvisc         | 0.0007301 | Paxs    | 414.25          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003870 | Paxs | 444.65 | Joback Method |
| dvisc | 0.0002225 | Paxs | 475.06 | Joback Method |
| dvisc | 0.0001368 | Paxs | 505.46 | Joback Method |
| dvisc | 0.0000888 | Paxs | 535.86 | Joback Method |
| dvisc | 0.0000604 | Paxs | 566.26 | 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=R256878&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R256878&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>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>mccvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-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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