

# Benzaldehyde, 2-hydroxy, 5-octyl

**Inchi:** InChI=1S/C15H22O2/c1-2-3-4-5-6-7-8-13-9-10-15(17)14(11-13)12-16/h9-12,17H,2-8H2,  
**InchiKey:** SXIFMUZENYUSFJ-UHFFFAOYSA-N  
**Formula:** C15H22O2  
**SMILES:** CCCCCCCCc1ccc(O)c(C=O)c1  
**Mol. weight [g/mol]:** 234.33

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -75.94  | kJ/mol  | Joback Method  |
| hf            | -390.76 | kJ/mol  | Joback Method  |
| hfus          | 36.33   | kJ/mol  | Joback Method  |
| hvap          | 71.66   | kJ/mol  | Joback Method  |
| log10ws       | -4.58   |         | Crippen Method |
| logp          | 4.108   |         | Crippen Method |
| mcvol         | 205.890 | ml/mol  | McGowan Method |
| pc            | 2227.09 | kPa     | Joback Method  |
| rinpol        | 2085.00 |         | NIST Webbook   |
| rinpol        | 2085.00 |         | NIST Webbook   |
| tb            | 703.54  | K       | Joback Method  |
| tc            | 908.87  | K       | Joback Method  |
| tf            | 451.47  | K       | Joback Method  |
| vc            | 0.750   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 577.10    | J/mol×K | 703.54          | Joback Method |
| cpg           | 644.32    | J/mol×K | 874.65          | Joback Method |
| cpg           | 632.20    | J/mol×K | 840.43          | Joback Method |
| cpg           | 619.49    | J/mol×K | 806.21          | Joback Method |
| cpg           | 606.12    | J/mol×K | 771.98          | Joback Method |
| cpg           | 592.01    | J/mol×K | 737.76          | Joback Method |
| cpg           | 655.92    | J/mol×K | 908.87          | Joback Method |
| dvisc         | 0.0000169 | Pa×s    | 703.54          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000252 | Pa×s | 661.53 | Joback Method |
| dvisc | 0.0000397 | Pa×s | 619.52 | Joback Method |
| dvisc | 0.0000666 | Pa×s | 577.50 | Joback Method |
| dvisc | 0.0001212 | Pa×s | 535.49 | Joback Method |
| dvisc | 0.0002444 | Pa×s | 493.48 | Joback Method |
| dvisc | 0.0005613 | Pa×s | 451.47 | 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>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=R256898&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R256898&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>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>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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