# Benzaldehyde, 2-hydroxy, 3,5-di(t-butyl)

**Other names:** 3,5-di-tert-butyl-2-hydroxybenzaldehyde
**Inchi:** InChI=1S/C15H22O2/c1-14(2,3)11-7-10(9-16)13(17)12(8-11)15(4,5)6/h7-9,17H,1-6H3
**InchiKey:** RRIQVLZDOZPJTH-UHFFFAOYSA-N
**Formula:** C15H22O2
**SMILES:** CC(C)(C)c1cc(C=O)c(O)c(C(C)(C)C)c1
**Mol. weight [g/mol]:** 234.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -79.89 | kJ/mol | Joback Method |
| hf | -419.73 | kJ/mol | Joback Method |
| hfus | 21.11 | kJ/mol | Joback Method |
| hvap | 69.73 | kJ/mol | Joback Method |
| log10ws | -3.89 | | Crippen Method |
| logp | 3.800 | | Crippen Method |
| mcvol | 205.890 | ml/mol | McGowan Method |
| pc | 2276.24 | kPa | Joback Method |
| rinpol | 1800.00 | | NIST Webbook |
| tb | 702.06 | K | Joback Method |
| tc | 930.12 | K | Joback Method |
| tf | 468.83 | K | Joback Method |
| vc | 0.729 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 663.43 | J/mol×K | 930.12 | Joback Method |
| cpg | 597.31 | J/mol×K | 740.07 | Joback Method |
| cpg | 612.03 | J/mol×K | 778.08 | Joback Method |
| cpg | 625.87 | J/mol×K | 816.09 | Joback Method |
| cpg | 638.96 | J/mol×K | 854.10 | Joback Method |
| cpg | 651.43 | J/mol×K | 892.11 | Joback Method |
| cpg | 581.56 | J/mol×K | 702.06 | Joback Method |
| dvisc | 0.0000179 | Pa×s | 663.19 | Joback Method |

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| dvisc | 0.0000282 | Pa×s | 624.32 | Joback Method |
| dvisc | 0.0000472 | Pa×s | 585.44 | Joback Method |
| dvisc | 0.0000850 | Pa×s | 546.57 | Joback Method |
| dvisc | 0.0001675 | Pa×s | 507.70 | Joback Method |
| dvisc | 0.0000120 | Pa×s | 702.06 | Joback Method |
| dvisc | 0.0003692 | Pa×s | 468.83 | Joback Method |
| psub | 2.37e-04 | kPa | 300.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 2.34e-04 | kPa | 300.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 3.22e-04 | kPa | 302.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 3.04e-04 | kPa | 302.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 3.00e-04 | kPa | 302.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 4.08e-04 | kPa | 304.15 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

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| psub | 2.48e-04 | kPa | 300.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 3.78e-04 | kPa | 304.15 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 5.42e-04 | kPa | 306.37 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 5.14e-04 | kPa | 306.37 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 5.05e-04 | kPa | 306.37 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 6.73e-04 | kPa | 308.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 6.31e-04 | kPa | 308.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

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|---|---|---|---|---|
| psub | 6.20e-04 | kPa | 308.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 8.61e-04 | kPa | 310.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 8.12e-04 | kPa | 310.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 8.01e-04 | kPa | 310.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.10e-03 | kPa | 312.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.03e-03 | kPa | 312.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.01e-03 | kPa | 312.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

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|---|---|---|---|---|
| psub | 1.76e-04 | kPa | 298.16 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.80e-04 | kPa | 298.16 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.93e-04 | kPa | 298.16 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.40e-04 | kPa | 296.28 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.43e-04 | kPa | 296.28 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.51e-04 | kPa | 296.28 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 3.82e-04 | kPa | 304.15 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

# Sources

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|---|---|
| **Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde:** | https://www.doi.org/10.1016/j.jct.2009.10.009 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R256818&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **psub:** | Sublimation pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |