

Benzaldehyde, 3-hydroxy-

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| Other names: | 3-Formylphenol 3-hydroxybenzaldehyde Benzaldehyde, m-hydroxy- m-Formylphenol m-Hydroxybenzaldehyde meta-Hydroxybenzaldehyde |
| Inchi: | InChI=1S/C7H6O2/c8-5-6-2-1-3-7(9)4-6/h1-5,9H |
| InchiKey: | IAVREABSGIHHMO-UHFFFAOYSA-N |
| Formula: | C7H6O2 |
| SMILES: | O=Cc1cccc(O)c1 |
| Mol. weight [g/mol]: | 122.12 |
| CAS: | 100-83-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|---------|---|
| gf | -133.67 | kJ/mol | Joback Method |
| hf | -214.17 | kJ/mol | Joback Method |
| hfus | 24.10 | kJ/mol | Synthesis and characterization of novel binary organic monotectic and eutectic alloys |
| hsub | 100.10 ± 0.60 | kJ/mol | NIST Webbook |
| hvap | 53.19 | kJ/mol | Joback Method |
| log10ws | -1.26 | | Crippen Method |
| logp | 1.205 | | Crippen Method |
| mcvol | 93.170 | ml/mol | McGowan Method |
| pc | 5602.57 | kPa | Joback Method |
| rinpol | 1267.00 | | NIST Webbook |
| rinpol | 1262.40 | | NIST Webbook |
| tb | 513.20 | K | NIST Webbook |
| tc | 749.54 | K | Joback Method |
| tf | 376.00 | K | Measurement and modeling for solubility of 3-hydroxybenzaldehyde and its mixture with 4-hydroxybenzaldehyde in supercritical carbon dioxide |
| vc | 0.302 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------------|---------|-----------------|--|
| cpg | 197.64 | J/molxK | 515.52 | Joback Method |
| cpg | 206.73 | J/molxK | 554.52 | Joback Method |
| cpg | 215.05 | J/molxK | 593.53 | Joback Method |
| cpg | 222.66 | J/molxK | 632.53 | Joback Method |
| cpg | 229.65 | J/molxK | 671.53 | Joback Method |
| cpg | 236.10 | J/molxK | 710.54 | Joback Method |
| cpg | 242.09 | J/molxK | 749.54 | Joback Method |
| dvisc | 0.0031017 | Paxs | 348.79 | Joback Method |
| dvisc | 0.0014153 | Paxs | 376.58 | Joback Method |
| dvisc | 0.0007194 | Paxs | 404.37 | Joback Method |
| dvisc | 0.0003989 | Paxs | 432.15 | Joback Method |
| dvisc | 0.0002375 | Paxs | 459.94 | Joback Method |
| dvisc | 0.0001500 | Paxs | 487.73 | Joback Method |
| dvisc | 0.0000996 | Paxs | 515.52 | Joback Method |
| hsubt | 99.70 ± 0.60 | kJ/mol | 321.00 | NIST Webbook |
| psub | 2.20e-04 | kPa | 316.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.34e-04 | kPa | 312.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.31e-04 | kPa | 312.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.77e-04 | kPa | 314.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

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|------|----------|-----|--------|--|
| psub | 1.71e-04 | kPa | 314.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.68e-04 | kPa | 314.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 2.33e-04 | kPa | 316.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.39e-04 | kPa | 312.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 2.16e-04 | kPa | 316.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 2.88e-04 | kPa | 318.19 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 2.80e-04 | kPa | 318.19 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

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|------|----------|-----|--------|--|
| psub | 2.75e-04 | kPa | 318.19 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 3.77e-04 | kPa | 320.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 3.58e-04 | kPa | 320.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 3.53e-04 | kPa | 320.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 4.62e-04 | kPa | 322.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 4.53e-04 | kPa | 322.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 4.40e-04 | kPa | 322.20 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

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|------|----------|-----|--------|--|
| psub | 5.81e-04 | kPa | 324.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 5.57e-04 | kPa | 324.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 5.42e-04 | kPa | 324.17 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 7.38e-04 | kPa | 326.22 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 7.12e-04 | kPa | 326.22 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 6.94e-04 | kPa | 326.22 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 9.07e-04 | kPa | 328.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

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|------|----------|-----|--------|--|
| psub | 8.71e-04 | kPa | 328.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 8.49e-04 | kPa | 328.18 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.14e-03 | kPa | 330.19 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.09e-03 | kPa | 330.19 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |
| psub | 1.06e-03 | kPa | 330.19 | Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 464.20 | K | 6.70 | NIST Webbook |

Sources

Synthesis and characterization of novel binary organic monotectic and eutectic alloys
 McGowan Method: <https://www.doi.org/10.1016/j.tca.2012.02.020>
<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C100834&Units=SI>

Thermodynamic study on hydroxybenzaldehyde derivatives: 3-methoxybenzaldehyde isomers <https://www.doi.org/10.1016/j.jct.2009.10.009>

Measurement and modeling of solubility of 3-hydroxybenzaldehyde <https://www.doi.org/10.1016/j.fluid.2015.10.012>

Joback Method with 9,9-difert-butyl-2-hydroxybenzaldehyde https://en.wikipedia.org/wiki/Joback_method

4-hydroxybenzaldehyde in supercritical carbon dioxide: Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Solubilities of hydroxybenzaldehyde isomers and their mixture in subcritical 1,1,1,2-tetrafluoroethane: <https://www.doi.org/10.1016/j.tca.2015.11.027>

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 |
| hsub: | Enthalpy of sublimation at standard conditions |
| hsubt: | Enthalpy of sublimation at a given temperature |
| 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 |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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