# Benzoic acid, 2,6-dihydroxy-

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| **Other names:** | 2,6-Resorcylic acid |
| | 2,6-dihydroxybenzoic acid |
| | 2-Carboxyresorcinol |
| | 6-Hydroxysalicylic acid |
| | «gamma»-Resorcylic acid |
| **Inchi:** | InChI=1S/C7H6O4/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3,8-9H,(H,10,11) |
| **InchiKey:** | AKEUNCKRJATALU-UHFFFAOYSA-N |
| **Formula:** | C7H6O4 |
| **SMILES:** | O=C(O)c1c(O)cccc1O |
| **Mol. weight [g/mol]:** | 154.12 |
| **CAS:** | 303-07-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -454.51 | kJ/mol | Joback Method |
| hf | -570.71 | kJ/mol | Joback Method |
| hfus | 25.00 | kJ/mol | Thermochemical study of 2,4-, 2,6- and 3,4-dihydroxybenzoic acids in the liquid phase using a TG apparatus |
| hsub | 109.10 ± 1.00 | kJ/mol | NIST Webbook |
| hvap | 82.90 | kJ/mol | Joback Method |
| log10ws | -0.63 | | Crippen Method |
| logp | 0.796 | | Crippen Method |
| mcvol | 104.910 | ml/mol | McGowan Method |
| pc | 8175.04 | kPa | Joback Method |
| rinpol | 1397.00 | | NIST Webbook |
| rinpol | 1397.00 | | NIST Webbook |
| tb | 693.53 | K | Joback Method |
| tc | 922.45 | K | Joback Method |
| tf | 440.20 | K | Measurement and Correlation of the Solubility of 2,6-Dihydroxybenzoic Acid in Alcohols and Binary Solvents |
| vc | 0.277 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 267.80 | J/mol×K | 693.53 | Joback Method |
| cpg | 279.67 | J/mol×K | 769.84 | Joback Method |
| cpg | 285.24 | J/mol×K | 807.99 | Joback Method |
| cpg | 273.90 | J/mol×K | 731.68 | Joback Method |
| cpg | 296.25 | J/mol×K | 884.30 | Joback Method |
| cpg | 290.73 | J/mol×K | 846.15 | Joback Method |
| cpg | 301.93 | J/mol×K | 922.45 | Joback Method |
| dvisc | 0.0000285 | Pa×s | 529.26 | Joback Method |
| dvisc | 0.0000136 | Pa×s | 556.64 | Joback Method |
| dvisc | 0.0000038 | Pa×s | 611.39 | Joback Method |
| dvisc | 0.0000021 | Pa×s | 638.77 | Joback Method |
| dvisc | 0.0000013 | Pa×s | 666.15 | Joback Method |
| dvisc | 0.0000008 | Pa×s | 693.53 | Joback Method |
| dvisc | 0.0000069 | Pa×s | 584.02 | Joback Method |
| hsubt | 107.50 ± 1.00 | kJ/mol | 356.00 | NIST Webbook |
| psub | 7.13e-04 | kPa | 363.19 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 4.79e-04 | kPa | 359.28 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 6.09e-04 | kPa | 361.38 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 5.90e-04 | kPa | 361.38 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 5.86e-04 | kPa | 361.38 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |

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| psub | 4.77e-04 | kPa | 359.28 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 6.92e-04 | kPa | 363.19 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 6.79e-04 | kPa | 363.19 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 8.81e-04 | kPa | 365.17 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 8.45e-04 | kPa | 365.17 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 8.34e-04 | kPa | 365.17 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 4.91e-04 | kPa | 359.28 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 3.86e-04 | kPa | 357.20 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 3.91e-04 | kPa | 357.20 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 4.01e-04 | kPa | 357.20 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |

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| psub | 3.23e-04 | kPa | 355.35 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 3.36e-04 | kPa | 355.35 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 2.49e-04 | kPa | 353.26 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 2.55e-04 | kPa | 353.26 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 2.08e-04 | kPa | 351.02 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 2.04e-04 | kPa | 351.02 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 1.73e-04 | kPa | 349.32 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 1.71e-04 | kPa | 349.32 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 1.33e-04 | kPa | 347.14 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |
| psub | 1.31e-04 | kPa | 347.14 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |

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| psub | 1.38e-04 | kPa | 347.14 | Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers |

# Sources

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| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C303071&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Thermochemical study of 2,4-, 2,6- and 3,4-dihydroxybenzoic acids in the liquid phase using a TG apparatus:** | https://www.doi.org/10.1016/j.tca.2011.01.001 |
| **Measurement and Correlation of the Solubility of 2,6-Dihydroxybenzoic Acid in Alcohols and Binary Solvents:** | https://www.doi.org/10.1021/acs.jced.6b00957 |
| **Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers:** | https://www.doi.org/10.1021/je900777q |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |