

Benzaldehyde, 4-hydroxy-

Other names:	4-Formylphenol
	4-Hydroxybenzaldehyde
	4-Hydroxybenzenecarbonal
	Benzaldehyde, p-hydroxy-
	NSC 2127
	P-HYDROXY BENZALDEHYDE
	Parahydroxybenzaldehyde
	USAF M-6
	p-Formylphenol
	p-Hydroxybenzaldehyde
	p-Oxybenzaldehyde
Inchi:	InChI=1S/C7H6O2/c8-5-6-1-3-7(9)4-2-6/h1-5,9H
InchiKey:	RGHHSNMVTDWUBI-UHFFFAOYSA-N
Formula:	C7H6O2
SMILES:	O=Cc1ccc(O)cc1
Mol. weight [g/mol]:	122.12
CAS:	123-08-0

Physical Properties

Property code	Value	Unit	Source
gf	-133.67	kJ/mol	Joback Method
hf	-214.17	kJ/mol	Joback Method
hfus	16.00	kJ/mol	Joback Method
hsub	102.50 ± 0.50	kJ/mol	NIST Webbook
hsub	99.70 ± 0.40	kJ/mol	NIST Webbook
hsub	98.20 ± 1.30	kJ/mol	NIST Webbook
hvap	53.19	kJ/mol	Joback Method
ie	9.32 ± 0.02	eV	NIST Webbook
log10ws	-0.96		Aqueous Solubility Prediction Method
log10ws	-0.96		Estimated Solubility Method
logp	1.205		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
rinpol	1308.00		NIST Webbook
rinpol	1311.00		NIST Webbook

rinpol	1317.00		NIST Webbook
rinpol	1320.80		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1318.60		NIST Webbook
rinpol	1324.00		NIST Webbook
ripol	2958.00		NIST Webbook
ripol	2958.00		NIST Webbook
tb	515.52	K	Joback Method
tc	749.54	K	Joback Method
tf	387.00	K	Measurement and modeling for solubility of 3-hydroxybenzaldehyde and its mixture with 4-hydroxybenzaldehyde in supercritical carbon dioxide
tf	390.48	K	Aqueous Solubility Prediction Method
vc	0.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.09	J/mol×K	749.54	Joback Method
cpg	206.73	J/mol×K	554.52	Joback Method
cpg	215.05	J/mol×K	593.53	Joback Method
cpg	222.66	J/mol×K	632.53	Joback Method
cpg	229.65	J/mol×K	671.53	Joback Method
cpg	236.10	J/mol×K	710.54	Joback Method
cpg	197.64	J/mol×K	515.52	Joback Method
dvisc	0.0001500	Paxs	487.73	Joback Method
dvisc	0.0002375	Paxs	459.94	Joback Method
dvisc	0.0003989	Paxs	432.15	Joback Method
dvisc	0.0007194	Paxs	404.37	Joback Method
dvisc	0.0014153	Paxs	376.58	Joback Method
dvisc	0.0000996	Paxs	515.52	Joback Method
dvisc	0.0031017	Paxs	348.79	Joback Method

hfust	20.30	kJ/mol	390.80	NIST Webbook
hfust	21.60	kJ/mol	390.80	NIST Webbook
hsubt	101.80 ± 0.50	kJ/mol	332.50	NIST Webbook
hsubt	91.20	kJ/mol	324.00	NIST Webbook
hvapt	72.30	kJ/mol	488.50	NIST Webbook
psub	1.49e-04	kPa	324.20	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	2.42e-04	kPa	328.31	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	3.08e-04	kPa	330.18	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	3.03e-04	kPa	330.18	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	2.96e-04	kPa	330.18	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.51e-04	kPa	324.20	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	3.75e-04	kPa	332.16	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

psub	3.70e-04	kPa	332.16	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	4.77e-04	kPa	334.18	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	4.72e-04	kPa	334.18	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	4.63e-04	kPa	334.18	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	6.03e-04	kPa	336.22	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	6.02e-04	kPa	336.22	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	5.83e-04	kPa	336.22	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

psub	7.56e-04	kPa	338.34	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	7.38e-04	kPa	338.34	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	7.28e-04	kPa	338.34	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	9.26e-04	kPa	340.17	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	9.05e-04	kPa	340.17	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	8.86e-04	kPa	340.17	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.02e-03	kPa	341.30	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

psub	1.01e-03	kPa	341.30	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	9.84e-04	kPa	341.30	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.57e-04	kPa	324.20	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	2.44e-04	kPa	328.31	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	2.52e-04	kPa	328.31	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.87e-04	kPa	326.16	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.93e-04	kPa	326.16	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

psub	1.97e-04	kPa	326.16	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	3.82e-04	kPa	332.16	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.33034e+01
Coeff. B	-1.08755e+04
Coeff. C	-6.35445e+00
Coeff. D	1.28665e-06
Temperature range (K), min.	390.15
Temperature range (K), max.	844.00

Sources

Solubilities of hydroxybenzaldehyde isomers and their mixture in subcritical CO₂/1,1,1,2-tetrafluoroethane: KDB

<https://www.doi.org/10.1016/j.tca.2015.11.027>

Measurement and modeling for solubility of 3-hydroxybenzaldehyde and 4-hydroxybenzaldehyde in supercritical carbon dioxide: Joback Method

<https://www.cheric.org/files/research/kdb/mol/mol1247.mol>

Solubility of 4-Hydroxybenzaldehyde in Supercritical Carbon Dioxide with and without Co-solvents: McGowan Method

<https://www.doi.org/10.1016/j.fluid.2015.10.012>

NIST Webbook:

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde: Aqueous Solubility Prediction Method

https://en.wikipedia.org/wiki/Joback_method

Thermodynamic Difference between Protocatechualdehyde and p-Hydroxybenzaldehyde in Aqueous Sodium Chloride Solutions:

<https://www.doi.org/10.1021/je401082x>

Solubility of 3-Hydroxybenzaldehyde in Supercritical Carbon Dioxide with and without Co-solvents: McGowan Method

<http://link.springer.com/article/10.1007/BF02311772>

Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C123080&Units=SI>

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>

Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

<https://www.doi.org/10.1021/acs.jced.6b00458>

KDB Vapor Pressure Data:<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1247>

**Determination and Modeling of
Solid-Liquid Equilibrium for Ternary
Systems of Terephthalaldehyde +
4-Hydroxybenzaldehyde + Ethyl
Acetate/Acetone:**

<https://www.doi.org/10.1021/acs.jced.8b00801>

Legend

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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