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	99.70 ± 0.40	kJ/mol	NIST Webbook
hsub	98.20 ± 1.30	kJ/mol	NIST Webbook
hsub	102.50 ± 0.50	kJ/mol	NIST Webbook
hvap	53.19	kJ/mol	Joback Method
ie	9.32 ± 0.02	eV	NIST Webbook
log10ws	-0.96		Estimated Solubility Method
log10ws	-0.96		Aqueous Solubility Prediction Method
logp	1.205		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
rinpol	1311.00		NIST Webbook
rinpol	1323.00		NIST Webbook

rinpol	1318.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1320.80		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1318.60		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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.10	J/mol×K	710.54	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	242.09	J/mol×K	749.54	Joback Method
cpg	197.64	J/mol×K	515.52	Joback Method
dvisc	0.0000996	Pa×s	515.52	Joback Method
dvisc	0.0002375	Pa×s	459.94	Joback Method
dvisc	0.0003989	Pa×s	432.15	Joback Method
dvisc	0.0014153	Pa×s	376.58	Joback Method
dvisc	0.0031017	Pa×s	348.79	Joback Method
dvisc	0.0007194	Pa×s	404.37	Joback Method
dvisc	0.0001500	Pa×s	487.73	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	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	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	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	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	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	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	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	4.77e-04	kPa	334.18	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	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	3.82e-04	kPa	332.16	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	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	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	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	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	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	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	1.57e-04	kPa	324.20	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(Pvp) = A + B/T + C*ln(T) + D*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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Solubility of 4-Hydroxybenzaldehyde in Supercritical Carbon Dioxide with and without Cosolvents:	https://www.doi.org/10.1021/je401082x
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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 Terephthaldehyde + Hydroxybenzaldehyde + Ethyl Acetate/Acetone:	https://www.doi.org/10.1021/acs.jced.8b00801
Thermodynamic study on hydroxybenzaldehyde derivatives: 3-Hydroxybenzaldehyde + Ethyl Acetate/Acetone:	https://www.doi.org/10.1016/j.jct.2009.10.009
Solubilities of hydroxybenzaldehyde isomers and their mixture in subcritical CO2: 2. tetrafluoromethane:	https://www.doi.org/10.1016/j.tca.2015.11.027
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1247.mol
3,5-di-tert-butyl-2-hydroxybenzaldehyde:	
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Measurement and modeling for solubility of 3-hydroxybenzaldehyde and its mixture with 4-hydroxybenzaldehyde in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2015.10.012
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123080&Units=SI

https://www.doi.org/10.1021/acs.jced.6b00458
http://pubs.acs.org/doi/abs/10.1021/ci990307l

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