Benzaldehyde, 3-hydroxy-

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	1262.40		NIST Webbook
rinpol	1267.00		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/mol×K	515.52	Joback Method
cpg	215.05	J/mol×K	593.53	Joback Method
cpg	222.66	J/mol×K	632.53	Joback Method
cpg	206.73	J/mol×K	554.52	Joback Method
cpg	236.10	J/mol×K	710.54	Joback Method
cpg	229.65	J/mol×K	671.53	Joback Method
cpg	242.09	J/mol×K	749.54	Joback Method
dvisc	0.0031017	Pa×s	348.79	Joback Method
dvisc	0.0014153	Pa×s	376.58	Joback Method
dvisc	0.0003989	Pa×s	432.15	Joback Method
dvisc	0.0002375	Pa×s	459.94	Joback Method
dvisc	0.0001500	Pa×s	487.73	Joback Method
dvisc	0.0000996	Pa×s	515.52	Joback Method
dvisc	0.0007194	Pa×s	404.37	Joback Method
hsubt	99.70 ± 0.60	kJ/mol	321.00	NIST Webbook
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	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
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	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	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
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
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	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	3.77e-04	kPa	320.18	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

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	2.80e-04	kPa	318.19	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	2.16e-04	kPa	316.20	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	2.20e-04	kPa	316.20	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	1.68e-04	kPa	314.20	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

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	1.77e-04	kPa	314.20	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	1.34e-04	kPa	312.17	Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.39e-04	kPa	312.17	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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Synthesis and characterization of novel binary organic monotectic and eutectic systems:	https://www.doi.org/10.1016/j.tca.2012.02.020
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
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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