

Benzoic acid, 3,4-dihydroxy-

Other names:	3,4-dihydroxybenzoic acid 4-Carboxy-1,2-dihydroxybenzene Protocatechuic acid protocatechoic acid
Inchi:	InChI=1S/C7H6O4/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3,8-9H,(H,10,11)
InchiKey:	YQUVCSBJEUQKSH-UHFFFAOYSA-N
Formula:	C7H6O4
SMILES:	O=C(O)c1ccc(O)c(O)c1
Mol. weight [g/mol]:	154.12
CAS:	99-50-3

Physical Properties

Property code	Value	Unit	Source
gf	-454.51	kJ/mol	Joback Method
hf	-570.71	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Thermochemical study of 2,4-, 2,6- and 3,4-dihydroxybenzoic acids in the liquid phase using a TG apparatus
hsub	135.10 ± 1.20	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	1557.00		NIST Webbook
rinpol	1557.00		NIST Webbook
tb	693.53	K	Joback Method
tc	922.45	K	Joback Method
tf	529.26	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	267.80	J/mol×K	693.53	Joback Method
cpg	273.90	J/mol×K	731.68	Joback Method
cpg	279.67	J/mol×K	769.84	Joback Method
cpg	285.24	J/mol×K	807.99	Joback Method
cpg	290.73	J/mol×K	846.15	Joback Method
cpg	296.25	J/mol×K	884.30	Joback Method
cpg	301.93	J/mol×K	922.45	Joback Method
dvisc	0.0000136	Pa×s	556.64	Joback Method
dvisc	0.0000285	Pa×s	529.26	Joback Method
dvisc	0.0000069	Pa×s	584.02	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
hfust	31.20	kJ/mol	472.30	NIST Webbook
hsubt	132.30 ± 1.20	kJ/mol	395.00	NIST Webbook
psub	8.60e-05	kPa	387.12	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	8.70e-05	kPa	387.12	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	8.90e-05	kPa	387.12	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	1.32e-04	kPa	391.31	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	1.33e-04	kPa	391.31	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	1.33e-04	kPa	391.31	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers

psub	1.66e-04	kPa	393.33	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	1.64e-04	kPa	393.33	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	1.65e-04	kPa	393.33	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.01e-04	kPa	395.20	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.00e-04	kPa	395.20	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.02e-04	kPa	395.20	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.49e-04	kPa	397.32	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.53e-04	kPa	397.32	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	2.50e-04	kPa	397.32	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	3.67e-04	kPa	401.25	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers

psub	3.67e-04	kPa	401.25	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	3.65e-04	kPa	401.25	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	4.51e-04	kPa	403.26	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	4.52e-04	kPa	403.26	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
psub	4.50e-04	kPa	403.26	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Separation of Protocatechuic Acid Using Di-(2-ethylhexyl)phosphoric Acid N-Isobutylphosphate, Toluene, and Petroleum Ether: Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers

<https://www.doi.org/10.1021/acs.jced.7b00797>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C99503&Units=SI>

<https://www.doi.org/10.1021/je900777q>

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

Solubility of Gallic Acid, Catechin, and Protocatechuic Acid in Subcritical Water from 293.15 to 318.15 K: Correlation of Solubility Data and Solubility of Gallic Acid, Vanillin, Syringic Acid, and Protocatechuic Acid in Aqueous Sulfate Solutions from (293.15 to 318.15) K: Thermochemical study of 2,4-, 2,6- and 3,4-dihydroxybenzoic acids in the liquid phase and salt addition affects on the solubility behaviour of some phenolic compounds and Correlation of Ethyl Vanillin Solubility in Different Binary Solvents at Temperatures from 273.15 to 313.15 K: Binary diffusion coefficients of phenolic compounds in subcritical water using a determination of peak enthalpies of solution and dissociation of protocatechuic acid in aqueous salt solutions by back-titration of alkali metal nitrate solutions from (293.15 to 318.15) K:

<https://www.doi.org/10.1021/je901097n>

<https://www.doi.org/10.1021/je500519y>

<https://www.doi.org/10.1021/je800205e>

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

<https://www.doi.org/10.1016/j.tca.2011.01.001>

<https://www.doi.org/10.1016/j.jct.2006.06.014>

<https://www.doi.org/10.1021/acs.jced.6b00972>

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

<https://www.doi.org/10.1016/j.fluid.2010.12.003>

<https://www.doi.org/10.1016/j.jct.2015.07.029>

<https://www.doi.org/10.1016/j.jct.2008.06.006>

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
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

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