

Hydroquinone

Other names:	1,4-Benzenediol
	1,4-Benzenediol (hydroquinone)
	1,4-Dihydroxy-benzeen
	1,4-Dihydroxy-benzol
	1,4-Dihydroxybenzen
	1,4-Dihydroxybenzene
	1,4-Diidrobenzene
	4-Hydroxyphenol
	Aida
	Arctuvín
	Benzene, p-dihydroxy-
	Benzohydroquinone
	Benzoquinol
	Black & White Bleaching Cream
	Black and White Bleaching Cream
	Derma-Blanch
	Diak 5
	Dihydroquinone
	Eldopacque
	Eldopaque
	Eldopaque forte
	Eldoquin
	Eldoquin forte
	HE 5
	Hidroquinone
	Hydrochinon
	Hydrochinone
	Hydroquinol
	Hydroquinole
	Idrochinone
	NCI-C55834
	Phiaquin
	Quinol
	Solaquin forte
	Tecquinol
	Tenox HQ
	Tequinol
	UN 2662
	USAF EK-356
	p-Benzenediol

p-Dihydroquinone
 p-Dihydroxybenzene
 p-Dioxobenzene
 p-Dioxybenzene
 p-Hydroquinone
 p-Hydroxyphenol
 p-quinol
Inchi: InChI=1S/C6H6O2/c7-5-1-2-6(8)4-3-5/h1-4,7-8H
InchiKey: QIGBRXMKCJKVMJ-UHFFFAOYSA-N
Formula: C6H6O2
SMILES: Oc1ccc(O)cc1
Mol. weight [g/mol]: 110.11
CAS: 123-31-9

Physical Properties

Property code	Value	Unit	Source
chs	-2847.50 ± 1.20	kJ/mol	NIST Webbook
chs	-2824.68	kJ/mol	NIST Webbook
chs	-2852.40 ± 0.88	kJ/mol	NIST Webbook
chs	-2855.60	kJ/mol	NIST Webbook
chs	-2865.00	kJ/mol	NIST Webbook
chs	-2856.00	kJ/mol	NIST Webbook
chs	-2861.00	kJ/mol	NIST Webbook
chs	-2858.00	kJ/mol	NIST Webbook
gf	-187.56	kJ/mol	Joback Method
hf	-268.90	kJ/mol	NIST Webbook
hf	-266.90	kJ/mol	NIST Webbook
hf	-268.40	kJ/mol	NIST Webbook
hf	-272.00	kJ/mol	NIST Webbook
hf	-277.00 ± 1.40	kJ/mol	NIST Webbook
hfs	-371.10 ± 1.30	kJ/mol	NIST Webbook
hfs	-362.50	kJ/mol	NIST Webbook
hfs	-361.00	kJ/mol	NIST Webbook
hfs	-363.00 ± 1.00	kJ/mol	NIST Webbook
hfs	-366.10 ± 1.20	kJ/mol	NIST Webbook
hfus	27.23	kJ/mol	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited

hfus	23.78	kJ/mol	Measurement of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behaviour of the bulk material in applications?
hsub	94.10	kJ/mol	NIST Webbook
hsub	94.10 ± 0.50	kJ/mol	NIST Webbook
hsub	99.20 ± 1.70	kJ/mol	NIST Webbook
hsub	94.13 ± 0.53	kJ/mol	NIST Webbook
hsub	103.76	kJ/mol	NIST Webbook
hvap	84.40 ± 0.70	kJ/mol	NIST Webbook
ie	8.44	eV	NIST Webbook
ie	7.95 ± 0.03	eV	NIST Webbook
ie	7.94 ± 0.01	eV	NIST Webbook
ie	7.93 ± 0.01	eV	NIST Webbook
ie	7.95 ± 0.05	eV	NIST Webbook
log10ws	-0.17		Estimated Solubility Method
log10ws	-0.17		Aqueous Solubility Prediction Method
logp	1.098		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
pc	7561.44	kPa	Joback Method
rinpol	1241.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	207.49		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	220.60		NIST Webbook
rinpol	220.60		NIST Webbook
ripol	2693.00		NIST Webbook
ripol	2693.00		NIST Webbook
ripol	2693.00		NIST Webbook
sg	343.10 ± 5.00	J/molxK	NIST Webbook
tb	558.20 ± 1.00	K	NIST Webbook
tb	558.20	K	NIST Webbook
tc	766.85	K	Joback Method
tf	445.00	K	NIST Webbook
tf	443.50 ± 0.30	K	NIST Webbook
tf	445.15	K	Liquid pharmaceuticals formulation by eutectic formation

tf	445.35	K	Aqueous Solubility Prediction Method
tf	445.00 ± 0.60	K	NIST Webbook
tf	445.00	K	Enthalpies of formation of dihydroxybenzenes revisited: Combining experimental and high-level ab initio data
tt	445.98 ± 0.03	K	NIST Webbook
tt	445.50 ± 0.30	K	NIST Webbook
vc	0.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.33	J/molxK	519.62	Joback Method
cpg	220.99	J/molxK	725.65	Joback Method
cpg	215.32	J/molxK	684.44	Joback Method
cpg	209.18	J/molxK	643.24	Joback Method
cpg	202.41	J/molxK	602.03	Joback Method
cpg	194.85	J/molxK	560.83	Joback Method
cpg	226.33	J/molxK	766.85	Joback Method
cps	133.50	J/molxK	297.90	NIST Webbook
cps	150.20	J/molxK	323.00	NIST Webbook
cps	130.50	J/molxK	274.30	NIST Webbook
cps	136.40	J/molxK	298.15	NIST Webbook
cps	131.90	J/molxK	298.15	NIST Webbook
cps	139.70	J/molxK	298.00	NIST Webbook
dvisc	0.0004493	Paxs	415.54	Joback Method
dvisc	0.0009603	Paxs	394.72	Joback Method
dvisc	0.0001210	Paxs	457.17	Joback Method
dvisc	0.0000684	Paxs	477.99	Joback Method
dvisc	0.0000251	Paxs	519.62	Joback Method
dvisc	0.0000406	Paxs	498.80	Joback Method
dvisc	0.0002260	Paxs	436.35	Joback Method
hfust	26.50	kJ/mol	444.95	NIST Webbook
hfust	27.23	kJ/mol	445.10	NIST Webbook
hfust	26.48	kJ/mol	453.00	NIST Webbook
hfust	27.11	kJ/mol	445.50	NIST Webbook
hfust	27.11	kJ/mol	445.10	NIST Webbook
hsubt	101.30	kJ/mol	370.50	NIST Webbook
hsubt	99.00 ± 2.00	kJ/mol	351.00	NIST Webbook
hsubt	103.80	kJ/mol	322.00	NIST Webbook

hsubt	103.80	kJ/mol	335.50	NIST Webbook
hsubt	100.60 ± 1.30	kJ/mol	332.00	NIST Webbook
hsubt	93.70 ± 0.50	kJ/mol	334.00	NIST Webbook
hsubt	104.00 ± 1.00	kJ/mol	342.00	NIST Webbook
hvapt	70.50	kJ/mol	503.50	NIST Webbook
psub	3.33e-04	kPa	339.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	3.53e-04	kPa	339.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.64e-04	kPa	337.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.62e-04	kPa	337.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.12e-04	kPa	335.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.17e-04	kPa	335.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.32e-04	kPa	335.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	2.75e-04	kPa	337.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.69e-04	kPa	333.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	5.56e-05	kPa	322.80	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	5.45e-05	kPa	322.80	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.72e-04	kPa	333.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.77e-04	kPa	333.10	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	5.13e-05	kPa	322.80	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	1.38e-04	kPa	331.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	3.40e-04	kPa	339.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.38e-04	kPa	331.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.05e-04	kPa	329.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.09e-04	kPa	329.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.13e-04	kPa	328.90	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	8.46e-05	kPa	326.90	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	8.72e-05	kPa	326.90	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	9.44e-05	kPa	326.90	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	6.93e-05	kPa	324.90	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	6.59e-05	kPa	324.80	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	7.43e-05	kPa	324.90	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.42e-04	kPa	331.10	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
rho1	1328.00	kg/m3	293.15	Measurements of Liquid Liquid Equilibria for the Quaternary System 2-Methoxy-2-methylpropane + Phenol + Hydroquinone + Water at 313.15 K

rhos	1338.00	kg/m3	298.15	Liquid liquid equilibria for the quaternary system methyl isobutyl ketone water phenol hydroquinone
rhos	1332.00	kg/m3	293.20	Ternary and Quaternary Liquid-Liquid Equilibria for Systems of Methyl Butyl Ketone + Water + Hydroquinone + Phenol at 313.2 K and Atmospheric Pressure
sfust	60.90	J/molxK	445.50	NIST Webbook
sfust	59.00	J/molxK	444.95	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	558.20	K	97.30	NIST Webbook
tbrp	558.00	K	97.30	NIST Webbook

Sources

Liquid pharmaceuticals formulation by eutectic formation: Joback Method: <https://www.doi.org/10.1016/j.fluid.2017.05.009>
https://en.wikipedia.org/wiki/Joback_method

Liquid-Liquid Equilibria for the Ternary System Methyl Isobutyl Ketone + Water + Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Experimental Data and Thermodynamic Modeling: Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Liquid-Liquid Equilibria for Ternary Systems: methyl isobutyl ketone + (catechol, resorcinol, and hydroquinone) for the quaternary system methyl isobutyl ketone + (catechol, resorcinol, and hydroquinone) + water. Different Solvents from 276.65 K to 345.10 K: Measurements and Thermodynamic Modeling of Liquid-Liquid Equilibria Data for Ternary and Quaternary Systems: methyl isopropyl ketone + (resorcinol or hydroquinone) + water systems at different temperatures. Combining experimental and high-level ab initio data: <https://www.doi.org/10.1021/je060245c>
<https://www.doi.org/10.1021/acs.jced.9b00506>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C123319&Units=SI>
<https://www.doi.org/10.1016/j.tca.2008.02.016>
<https://www.doi.org/10.1016/j.fluid.2016.11.005>
<https://www.doi.org/10.1016/j.fluid.2007.05.026>
<https://www.doi.org/10.1021/je0502748>
<https://www.doi.org/10.1021/acs.jced.9b00633>
<https://www.doi.org/10.1016/j.fluid.2016.08.040>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>
<https://www.doi.org/10.1021/je800307g>
<https://www.doi.org/10.1016/j.jct.2013.10.032>

Measurements of Liquid Liquid Equilibria for the Quaternary System 2-Methoxy-2-methylpropane + Phenol + Hydroquinone + Water at 313.15 K: Measurement of enthalpy curves of phase change materials via DSC and Liquid-Liquid Equilibria for Ternary (Method for separating the hydroquinone, phenol and quaternary liquids-liquid equilibria) 2015 was for Methyl Butyl Ketone + water + hydroquinone of several phenolics and Polyhydric Phosphoric acid for the same reason. mentioned behaviour of solutes: Apparent molar volumes and isentropic compression of catechol, resorcinol, and hydroquinone in aqueous solution at T = 292.15, 293.15, 298.15, 303.15, and 308.15 K.

3.31

<https://www.doi.org/10.1021/acs.jced.6b00349>
<http://link.springer.com/article/10.1007/BF02311772>
<https://www.doi.org/10.1021/je500532v>
<https://www.doi.org/10.1016/j.jct.2018.08.041>
http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
<https://www.doi.org/10.1021/je400488x>
<https://www.cheric.org/files/research/kdb/mol/mol864.mol>
<https://www.doi.org/10.1016/j.tca.2014.09.022>
<https://www.doi.org/10.1021/acs.jced.7b01127>
<https://www.doi.org/10.1021/acs.jced.5b00918>
<https://www.doi.org/10.1021/je050293h>
<https://www.doi.org/10.1016/j.ict.2010.04.018>

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
rho:	Liquid Density
rhos:	Solid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sq:	Molar entropy at standard conditions

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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