1,2-Benzenediol

Other names:	1,2-Benzenediol (pyrocatechol) 1,2-Dihydroxybenzene 2-Hydroxyphenol 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,(2R-trans)- Benzene, o-dihydroxy- CATECHOL Catechol (phenol) Durafur developer c Fouramine pch Fourrine 68 Kachin Katechol NCI-C55856 NSC 1573 O-DIHYDROXYBENZENE Oxyphenic acid PYROCATECHOL Pelagol grey c Phthalhydroquinone Pyrocatechin Pyrocatechine Pyrokatechin Pyrokatechol benzene, 1,2-dihydroxy- c.i. 76500 c.i. Oxidation base 26 o-Benzenediol o-Dioxybenzene o-Diphenol o-Hydroquinone o-Hydroxyphenol o-Phenylenediol o-catecol
Inchi:	InChI=1S/C6H6O2/c7-5-3-1-2-4-6(5)8/h1-4,7-8H
InchiKey:	YCIMNLLNPGFGHC-UHFFFAOYSA-N
Formula:	C6H6O2
SMILES:	Oc1ccccc1O
Mol. weight [g/mol]:	110.11
CAS:	120-80-9

Physical Properties

Property code	Value	Unit	Source
chs	-2862.00	kJ/mol	NIST Webbook
chs	-2865.49 ± 0.74	kJ/mol	NIST Webbook
chs	-2874.00	kJ/mol	NIST Webbook
chs	-2856.30 ± 1.10	kJ/mol	NIST Webbook
chs	-2864.50 ± 0.80	kJ/mol	NIST Webbook
gf	-187.56	kJ/mol	Joback Method
hf	-267.50 ± 1.90	kJ/mol	NIST Webbook
hf	-274.80 ± 1.20	kJ/mol	NIST Webbook
hf	-271.60 ± 2.00	kJ/mol	NIST Webbook
hf	-262.50	kJ/mol	NIST Webbook
hfs	-354.10 ± 1.10	kJ/mol	NIST Webbook
hfs	-344.00	kJ/mol	NIST Webbook
hfs	-353.10 ± 1.10	kJ/mol	NIST Webbook
hfs	-362.30 ± 1.10	kJ/mol	NIST Webbook
hfus	22.87	kJ/mol	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
hsub	86.60 ± 1.60	kJ/mol	NIST Webbook
hsub	86.60	kJ/mol	NIST Webbook
hsub	81.50	kJ/mol	NIST Webbook
hsub	87.50 ± 0.29	kJ/mol	NIST Webbook
hsub	87.50	kJ/mol	NIST Webbook
hsub	87.50 ± 0.30	kJ/mol	NIST Webbook
hsub	86.60 ± 1.60	kJ/mol	NIST Webbook
hvap	71.90 ± 0.80	kJ/mol	NIST Webbook
ie	8.56	eV	NIST Webbook
ie	8.15	eV	NIST Webbook
log10ws	0.62		Estimated Solubility Method
log10ws	0.62		Aqueous Solubility Prediction Method
logp	1.098		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
pc	7561.44	kPa	Joback Method
rinpol	1215.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1199.80		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1197.00		NIST Webbook

rinpol	1210.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1197.00		NIST Webbook
ripol	2657.00		NIST Webbook
ripol	2661.00		NIST Webbook
tb	518.20	K	NIST Webbook
tb	519.05 ± 0.50	K	NIST Webbook
tb	518.80 ± 0.40	K	NIST Webbook
tb	518.75	K	KDB
tb	513.00	K	NIST Webbook
tc	766.85	K	Joback Method
tf	377.00	K	Enthalpies of formation of dihydroxybenzenes revisited: Combining experimental and high-level ab initio data
tf	377.70 ± 0.10	K	NIST Webbook
tf	376.90 ± 0.30	K	NIST Webbook
tf	378.85	K	Liquid Liquid Equilibria for the Ternary System Methyl Isobutyl Ketone + 1,2-Benzenediol + Water
tf	378.15	K	Liquid pharmaceuticals formulation by eutectic formation
tf	378.35	K	Aqueous Solubility Prediction Method
tf	378.00	K	NIST Webbook
tf	378.00 ± 1.00	K	NIST Webbook
tf	376.55 ± 0.50	K	NIST Webbook
tf	376.35 ± 0.50	K	NIST Webbook
tf	377.15	K	KDB
tt	377.50 ± 0.20	K	NIST Webbook
vc	0.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.33	J/mol×K	766.85	Joback Method
cpg	215.32	J/mol×K	684.44	Joback Method
cpg	209.18	J/mol×K	643.24	Joback Method
cpg	202.41	J/mol×K	602.03	Joback Method
cpg	194.85	J/mol×K	560.83	Joback Method
cpg	186.33	J/mol×K	519.62	Joback Method

cpg	220.99	J/mol×K	725.65	Joback Method
cps	140.17	J/mol×K	298.15	NIST Webbook
cps	139.30	J/mol×K	297.90	NIST Webbook
cps	156.90	J/mol×K	323.00	NIST Webbook
cps	132.20	J/mol×K	298.00	NIST Webbook
cps	140.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0000251	Pa×s	519.62	Joback Method
dvisc	0.0009603	Pa×s	394.72	Joback Method
dvisc	0.0000684	Pa×s	477.99	Joback Method
dvisc	0.0002260	Pa×s	436.35	Joback Method
dvisc	0.0001210	Pa×s	457.17	Joback Method
dvisc	0.0000406	Pa×s	498.80	Joback Method
dvisc	0.0004493	Pa×s	415.54	Joback Method
hfust	22.76	kJ/mol	377.50	NIST Webbook
hfust	22.76	kJ/mol	337.50	NIST Webbook
hfust	22.01	kJ/mol	376.90	NIST Webbook
hfust	18.55	kJ/mol	377.60	NIST Webbook
hfust	22.87	kJ/mol	377.60	NIST Webbook
hfust	22.00	kJ/mol	376.85	NIST Webbook
hfust	22.01	kJ/mol	376.90	NIST Webbook
hfust	22.54	kJ/mol	377.70	NIST Webbook
hsubt	81.00 ± 2.00	kJ/mol	309.00	NIST Webbook
hsubt	80.00 ± 0.50	kJ/mol	302.50	NIST Webbook
hvapt	61.20	kJ/mol	408.50	NIST Webbook
hvapt	63.10	kJ/mol	457.00	NIST Webbook
psub	8.69e-04	kPa	308.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	8.03e-04	kPa	307.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	8.52e-04	kPa	308.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	2.19e-04	kPa	295.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.32e-04	kPa	295.90	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.37e-04	kPa	296.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	9.90e-04	kPa	309.80	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.44e-04	kPa	296.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.73e-04	kPa	297.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	3.01e-04	kPa	298.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	2.98e-04	kPa	298.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method	
psub	3.47e-04	kPa	299.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method	
psub	3.72e-04	kPa	300.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method	
psub	3.79e-04	kPa	300.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method	
psub	4.23e-04	kPa	301.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method	
psub	4.68e-04	kPa	302.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method	
psub	4.63e-04	kPa	302.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method	

psub	5.43e-04	kPa	303.50	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	5.77e-04	kPa	304.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	5.83e-04	kPa	304.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	6.57e-04	kPa	305.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	7.19e-04	kPa	306.10	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	6.98e-04	kPa	306.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.42e-04	kPa	296.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

pvap	742.90	kPa	621.80	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	4007.00	kPa	753.50	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	2997.00	kPa	727.90	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	81.47	kPa	511.30	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	147.00	kPa	535.70	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	187.40	kPa	547.00	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	349.10	kPa	577.60	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method

pvap	487.90	kPa	595.60	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	499.40	kPa	597.30	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	3993.00	kPa	754.80	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	988.90	kPa	640.10	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	992.80	kPa	640.90	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	1995.00	kPa	692.70	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	1996.00	kPa	692.70	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method

pvap	2496.00	kPa	711.50	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
pvap	2993.00	kPa	727.50	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
rhos	1346.00	kg/m3	298.15	Liquid Liquid Equilibria for the Ternary System n-Butyl Acetate + Pyrocatechol + Water at Different Temperatures at 101.3 kPa
sfust	60.30	J/mol×K	337.50	NIST Webbook
sfust	58.00	J/mol×K	376.85	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	412.20	K	2.95	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
tbp	418.60	K	3.93	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry

tbp	423.80	K	4.93	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.80971e+01
Coeff. B	-7.00435e+03
Coeff. C	1.50900e+00
Temperature range (K), min.	377.60
Temperature range (K), max.	546.32

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.05944e+02
Coeff. B	-1.15782e+04
Coeff. C	-1.29321e+01
Coeff. D	6.78528e-06
Temperature range (K), min.	377.60
Temperature range (K), max.	764.00

Sources

Liquid-Liquid Equilibrium of Water + 2-Methoxyphenol + Methyl Isobutyl Ketone and Water + 1,2-Benzenediol + Methyl Isobutyl Ketone at 303.15 K and 328.15 K:	https://www.doi.org/10.1021/acs.jced.7b00887
Liquid-liquid equilibrium for ternary systems methyl isobutyl ketone + guaiacol, resorcinol and hydroquinone) + water at 333.15 K, 343.15 K and 353.15 K:	https://www.doi.org/10.1016/j.fluid.2016.11.005
Extraction of phenolic compounds from aqueous solution using choline bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.fluid.2017.04.022
QSPR:	https://www.cheric.org/files/research/kdb/mol/mol862.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Solubilities of resorcinol and pyrocathecol and their mixture in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.tca.2011.04.002
Effects of structural isomerism on solution behaviour of solutes:	https://www.doi.org/10.1016/j.jct.2010.04.018
Liquid Liquid Equilibria for the Ternary System n-Butyl Acetate + Pyrocatechol + Water at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.6b00280
Measurements for Four Compounds by Liquid Chromatography Combined with Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je0602465
Liquid Liquid Equilibria for the Ternary System Methyl Isobutyl Ketone + 1,2-Benzenediol + Water at 298.2, 318.2, and 333.2 K:	https://www.doi.org/10.1016/j.fluid.2017.05.009
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=862
Measurements and Thermodynamic Modeling of Liquid-Liquid Equilibria for the Ternary Methyl Propyl Ketone + Catechol/Resorcinol/Hydroquinone + Water at 333.15 K, 343.15 K and 353.15 K:	https://www.doi.org/10.1021/acs.jced.9b00633
Experimental result and data correlation of liquid-liquid equilibrium for the ternary methyl propyl ketone + catechol + water at 333.15 K:	https://www.doi.org/10.1016/j.jct.2018.08.041
Gilpin Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Missenard Method:	http://link.springer.com/article/10.1007/BF02311772
Phase equilibria of phenolic compounds in water or ethanol:	https://www.doi.org/10.1016/j.fluid.2017.09.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal melting points by differential scanning calorimetry:	https://www.doi.org/10.1016/j.jct.2019.03.008
Dihydroxybenzenes: Catechol, Resorcinol and Hydroquinone: Revisited:	https://www.doi.org/10.1016/j.tca.2008.02.016
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120809&Units=SI
Liquid Liquid Equilibria for Octan-2-one + Dihydroxybenzene + Water at Different Temperatures: Experimental Data and Thermodynamic Modeling:	https://www.doi.org/10.1021/acs.jced.9b00506
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method:	https://www.doi.org/10.1021/je050293h
Liquid Liquid Equilibria for the Ternary System Methyl Isobutyl Ketone + 1,2-Benzenediol + Water:	https://www.doi.org/10.1021/je5005559
Liquid–Liquid Equilibrium for Ternary Systems of 2-Pentanone/Mesityl Oxide + Catechol + Water at 298.2, 318.2, and 333.2 K:	https://www.doi.org/10.1021/acs.jced.8b00380
Enthalpies of formation of dihydroxybenzenes revisited: Combining experimental and high-level ab initio data:	https://www.doi.org/10.1016/j.jct.2013.10.032

Legend

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
pvap:	Vapor pressure
rhos:	Solid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume