Resorcinol

Other names:	1,3-Benzenediol
	1,3-Dihydroxybenzene
	1,3-Dihydroxybenzene (resorcinol)
	3-HYDROXYPHENOL
	Benzene, 1,3-dihydroxy-
	Benzene, m-dihydroxy-
	C.I. 76505
	C.I. Developer 4
	C.I. Oxidation Base 31
	Developer O
	Developer R
	Developer RS
	Durafur Developer G
	Fouramine RS
	Fourrine 79
	Fourrine EW
	M-DIHYDROXYBENZENE
	NCI-C05970
	NSC 1571
	Nako TGG
	Pelagol Grey RS
	Pelagol RS
	Phenol, m-hydroxy-
	Rcra waste number U201
	Resorcin
	Resorcine
	Rodol RS
	UN 2876
	m-Benzenediol
	m-Dioxybenzene
	m-Hydroquinone
	m-Hydroxyphenol
	«alpha»-Resorcinol
	Â«alphaÂ»-Resorcinol
Inchi:	InChI=1S/C6H6O2/c7-5-2-1-3-6(8)4-5/h1-4,7-8H
InchiKey:	GHMLBKRAJCXXBS-UHFFFAOYSA-N
Formula:	C6H6O2
SMILES:	Oc1cccc(O)c1
Mol. weight [g/mol]:	110.11
CAS:	108-46-3

Physical Properties

Property code	Value	Unit	Source
affp	856.40	kJ/mol	NIST Webbook
chs	-2847.90 ± 1.10	kJ/mol	NIST Webbook
chs	-2861.00	kJ/mol	NIST Webbook
chs	-2867.00	kJ/mol	NIST Webbook
chs	-2850.60 ± 0.42	kJ/mol	NIST Webbook
ep	-15.00	J/mol×K	NIST Webbook
gf	-187.56	kJ/mol	Joback Method
hf	-284.70 ± 1.20	kJ/mol	NIST Webbook
hf	-265.20	kJ/mol	NIST Webbook
hf	-275.00	kJ/mol	NIST Webbook
hfs	-370.70 ± 1.10	kJ/mol	NIST Webbook
hfs	-351.20	kJ/mol	NIST Webbook
hfs	-368.00 ± 0.50	kJ/mol	NIST Webbook
hfus	17.29	kJ/mol	Joback Method
hsub	86.00 ± 0.52	kJ/mol	NIST Webbook
hsub	86.00	kJ/mol	NIST Webbook
hsub	87.50 ± 0.50	kJ/mol	NIST Webbook
hsub	93.00	kJ/mol	NIST Webbook
hvap	78.40 ± 1.30	kJ/mol	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.63	eV	NIST Webbook
log10ws	0.81		Aqueous Solubility Prediction Method
log10ws	0.81		Estimated Solubility Method
logp	1.098		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	6240.00	kPa	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
rinpol	216.79		NIST Webbook
rinpol	219.64		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	213.50		NIST Webbook
rinpol	213.50		NIST Webbook
rinpol	1368.00		NIST Webbook

rinpol	1368.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1368.00		NIST Webbook
tb	550.00	K	NIST Webbook
tb	549.10 ± 0.40	K	NIST Webbook
tb	554.55 ± 0.50	K	NIST Webbook
tb	549.05	K	KDB
tc	766.85	K	Joback Method
tf	383.90	K	Aqueous Solubility Prediction Method
tf	383.15	K	Liquid pharmaceuticals formulation by eutectic formation
tf	382.00	K	Enthalpies of formation of dihydroxybenzenes revisited: Combining experimental and high-level ab initio data
tf	382.85	K	KDB
tf	383.65	K	Thermal, physicochemical and microstructural studies of organic analog of nonmetal-nonmetal monotectic alloy
tt	383.54 ± 0.02	K	NIST Webbook
tt	382.80 ± 0.25	K	NIST Webbook
tt	382.70 ± 0.20	K	NIST Webbook
vc	0.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.18	J/mol×K	643.24	Joback Method
cpg	226.33	J/mol×K	766.85	Joback Method
cpg	220.99	J/mol×K	725.65	Joback Method
cpg	215.32	J/mol×K	684.44	Joback Method
cpg	194.85	J/mol×K	560.83	Joback Method
cpg	202.41	J/mol×K	602.03	Joback Method
cpg	186.33	J/mol×K	519.62	Joback Method
cps	151.00	J/mol×K	323.00	NIST Webbook
cps	131.00	J/mol×K	298.00	NIST Webbook
cps	131.40	J/mol×K	297.90	NIST Webbook
cps	135.53	J/mol×K	298.15	NIST Webbook
cps	139.30	J/mol×K	298.15	NIST Webbook

dvisc	0.0009603	Pa×s	394.72	Joback Method
dvisc	0.0001210	Pa×s	457.17	Joback Method
dvisc	0.0000684	Pa×s	477.99	Joback Method
dvisc	0.0000406	Pa×s	498.80	Joback Method
dvisc	0.0004493	Pa×s	415.54	Joback Method
dvisc	0.0000251	Pa×s	519.62	Joback Method
dvisc	0.0002260	Pa×s	436.35	Joback Method
hfust	18.90	kJ/mol	382.60	NIST Webbook
hfust	21.30	kJ/mol	382.80	NIST Webbook
hfust	21.30	kJ/mol	382.90	NIST Webbook
hfust	1.20	kJ/mol	366.80	NIST Webbook
hfust	18.90	kJ/mol	382.60	NIST Webbook
hfust	20.50	kJ/mol	381.00	NIST Webbook
hsubt	92.30	kJ/mol	353.50	NIST Webbook
hsubt	93.00 ± 21.00	kJ/mol	329.50	NIST Webbook
hsubt	93.40	kJ/mol	303.00	NIST Webbook
hsubt	95.00 ± 1.00	kJ/mol	329.00	NIST Webbook
hsubt	85.30 ± 0.50	kJ/mol	334.00	NIST Webbook
hvapt	74.30	kJ/mol	427.50	NIST Webbook
hvapt	74.30	kJ/mol	484.50	NIST Webbook
psub	9.66e-04	kPa	331.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	8.81e-04	kPa	330.10	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	7.74e-04	kPa	329.10	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited

psub	1.06e-03	kPa	332.10	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	1.24e-03	kPa	333.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	6.17e-04	kPa	326.70	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	1.47e-03	kPa	335.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	1.86e-03	kPa	337.10	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	2.23e-03	kPa	339.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	2.54e-03	kPa	340.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited

psub	2.72e-03	kPa	341.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	2.71e-03	kPa	341.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	3.40e-03	kPa	343.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	3.41e-03	kPa	343.50	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	3.54e-03	kPa	344.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	3.67e-03	kPa	344.40	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	4.58e-03	kPa	346.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited

psub	4.68e-03	kPa	346.40	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	5.53e-03	kPa	348.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	5.56e-03	kPa	348.40	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	5.69e-03	kPa	349.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	6.49e-03	kPa	350.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	6.43e-03	kPa	350.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	7.32e-03	kPa	351.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited

psub	7.73e-03	kPa	352.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	8.71e-03	kPa	353.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	9.84e-03	kPa	354.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	0.01	kPa	355.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	5.48e-04	kPa	326.10	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	0.01	kPa	357.40	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	0.01	kPa	358.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited

psub	0.01	kPa	358.60	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	0.02	kPa	360.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	4.00e-04	kPa	323.10	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	0.02	kPa	361.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	0.02	kPa	364.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	0.01	kPa	356.30	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
psub	1.34e-03	kPa	334.20	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited

psub	0.02	kPa	360.40	Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited
sfust	49.41	J/mol×K	382.60	NIST Webbook
sfust	3.27	J/mol×K	366.80	NIST Webbook
sfust	55.60	J/mol×K	382.80	NIST Webbook
sfust	53.80	J/mol×K	381.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	444.70	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	451.30	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	456.80	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
tbrp	451.20	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.64521e+02
Coeff. B	-1.68432e+04
Coeff. C	-2.08308e+01
Coeff. D	7.18739e-06
Temperature range (K), min.	382.00
Temperature range (K), max.	810.00

Sources

Liquid Liquid Equilibria for the Ternary System Methyl Isobutyl Ketone + Benzene-1,3-diol + Water	https://www.doi.org/10.1021/je5003048
Liquid-liquid equilibrium for ternary systems, methyl isobutyl ketone + (catechol, resorcinol and hydroquinone) + water at 333.15 K, 348.15 K and 353.15 K:	https://www.doi.org/10.1016/j.fluid.2016.11.005
Solubilities of resorcinol and pyrocatechol and their mixtures in subcritical carbon dioxide:	https://www.doi.org/10.1016/j.tca.2011.04.002
KDB:	https://www.cheric.org/files/research/kdb/mol/mol863.mol
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
Densities and Viscosities of Binary Solutions of Benzene-1,3-diol + Water, Ethanol + Propan-1-ol, and Butan-1-ol at T = (293.15 to 333.15) K:	https://www.doi.org/10.1021/je101173w
Thermal, physicochemical and micro-structural studies of organic analog of nonmetal-nonmetal (Molecule-Metal):	https://www.doi.org/10.1016/j.tca.2009.10.010
Measurements and Thermodynamic Modeling of Liquid-Liquid Equilibria for Ternary (Methyl Propyl Ketone + Catechol/Resorcinol/Hydroquinone + Water) Systems:	https://www.doi.org/10.1021/acs.jced.9b00633
Data for the Ternary (Methyl Propyl Ketone + Water) Systems at 313.15 K, 323.15 K, 333.15 K, and 343.15 K:	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
Di-Hydroxybenzenes: Catechol, Resorcinol, and Hydroquinone. Enthalpies of Phase Transitions Revisited:	https://www.doi.org/10.1016/j.tca.2008.02.016
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
Liquid pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1016/j.fluid.2017.05.009
Ternary liquid-liquid equilibria for methyl isopropyl ketone + (resorcinol or hydroquinone) + water systems at different temperatures:	https://www.doi.org/10.1016/j.fluid.2016.08.040
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=863
Liquid-Liquid Equilibria for Ternary (Methyl Propyl Ketone + Hydroquinone or Resorcinol + Water) Systems at 298.15 K, 313.15 K, and 333.15 K:	https://www.doi.org/10.1021/acs.jced.7b01127
Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry:	https://www.doi.org/10.1016/j.jct.2019.03.008
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental result and data correlation of liquid-liquid equilibrium for methyl isopropyl ketone + o, m, p-dihydroxybenzene + water at 333.15 K, 343.15 K and 353.15 K:	https://www.doi.org/10.1016/j.jct.2018.08.041
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108463&Units=SI
Effects of structural isomerism on solution behaviour of solutes: Apparent molar volumes and isentropic compression of catechol, resorcinal, and hydroquinone in aqueous solution at T = (283.15, 293.15, 298.15, 303.15, and 313.15) K:	https://www.doi.org/10.1016/j.jct.2010.04.018

Partial Molar Volumes and Viscosity B-Coefficients of Nicotinamide in Aqueous Resorcinol Solutions at T = (298.15, 308.15, and 318.15) K https://www.doi.org/10.1007/s10765-009-0567-5

Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method: https://www.doi.org/10.1021/je0602465

Legend

affp:	Proton affinity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ep:	Protonation entropy at 298K
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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume