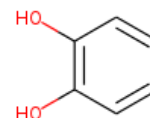


# 1,2-Benzenediol

**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; Oxyphenic acid; Pelagol grey c; Phthalhydroquinone; Pyrocatechin; Pyrocatechine; Pyrocatechol; Pyrokatechin; Pyrokatechol; c.i. 76500; c.i. Oxidation base 26; o-Benzenediol; o-Dihydroxybenzene; 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

**InChI Key:** YCIMNLLNPGFGHC-UHFFFAOYSA-N

**Formula:** C6H6O2

**SMILES:** Oc1ccccc1O

**Molecular Weight:** 110.11

**CAS:** 120-80-9

## Physical Properties

Property	Value	Unit	Source
$\Delta_c H^\circ_{\text{solid}}$	-2856.30 ± 1.10	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{solid}}$	-2864.50 ± 0.80	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{solid}}$	-2865.49 ± 0.74	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{solid}}$	-2874.00	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{solid}}$	-2862.00	kJ/mol	NIST Webbook
$\Delta_f G^\circ$	-187.56	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-274.80 ± 1.20	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{gas}}$	-267.50 ± 1.90	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{gas}}$	-271.60 ± 2.00	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{gas}}$	-262.50	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{solid}}$	-362.30 ± 1.10	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{solid}}$	-354.10 ± 1.10	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{solid}}$	-353.10 ± 1.10	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{solid}}$	-344.00	kJ/mol	NIST Webbook
$\Delta_{\text{fus}} H^\circ$	17.29	kJ/mol	Joback Method

Property	Value	Unit	Source
$\Delta_{\text{sub}} H^\circ$	87.50 ± 0.29	kJ/mol	NIST Webbook
$\Delta_{\text{sub}} H^\circ$	87.50	kJ/mol	NIST Webbook
$\Delta_{\text{sub}} H^\circ$	87.50 ± 0.30	kJ/mol	NIST Webbook
$\Delta_{\text{sub}} H^\circ$	86.60 ± 1.60	kJ/mol	NIST Webbook
$\Delta_{\text{sub}} H^\circ$	86.60 ± 1.60	kJ/mol	NIST Webbook
$\Delta_{\text{sub}} H^\circ$	86.60	kJ/mol	NIST Webbook
$\Delta_{\text{sub}} H^\circ$	81.50	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	71.90 ± 0.80	kJ/mol	NIST Webbook
IE	8.15	eV	NIST Webbook
IE	8.56	eV	NIST Webbook
$\log P_{\text{oct/wat}}$	1.098		Crippen Method
$P_c$	7561.44	kPa	Joback Method
$T_{\text{boil}}$	518.20	K	NIST Webbook
$T_{\text{boil}}$	513.00	K	NIST Webbook
$T_{\text{boil}}$	518.80 ± 0.40	K	NIST Webbook
$T_{\text{boil}}$	519.05 ± 0.50	K	NIST Webbook
$T_c$	766.85	K	Joback Method
$T_{\text{fus}}$	376.90 ± 0.30	K	NIST Webbook
$T_{\text{fus}}$	377.70 ± 0.10	K	NIST Webbook
$T_{\text{fus}}$	378.00	K	NIST Webbook
$T_{\text{fus}}$	378.00 ± 1.00	K	NIST Webbook
$T_{\text{fus}}$	376.55 ± 0.50	K	NIST Webbook
$T_{\text{fus}}$	376.35 ± 0.50	K	NIST Webbook
$T_{\text{triple}}$	377.50 ± 0.20	K	NIST Webbook
$V_c$	0.196	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	186.33	J/mol×K	519.62	Joback Method
$C_{p,solid}$	139.30	J/mol×K	297.9	NIST Webbook
$C_{p,solid}$	132.20	J/mol×K	298.0	NIST Webbook
$C_{p,solid}$	140.17	J/mol×K	298.15	NIST Webbook
$C_{p,solid}$	140.60	J/mol×K	298.15	NIST Webbook
$C_{p,solid}$	156.90	J/mol×K	323.0	NIST Webbook
$\eta$	0.0000251	Paxs	519.62	Joback Method
$\Delta_{fus} H$	22.76	kJ/mol	337.5	NIST Webbook
$\Delta_{fus} H$	22.00	kJ/mol	376.85	NIST Webbook
$\Delta_{fus} H$	22.01	kJ/mol	376.9	NIST Webbook
$\Delta_{fus} H$	22.01	kJ/mol	376.9	NIST Webbook
$\Delta_{fus} H$	22.76	kJ/mol	377.5	NIST Webbook
$\Delta_{fus} H$	22.87	kJ/mol	377.6	NIST Webbook
$\Delta_{fus} H$	18.55	kJ/mol	377.6	NIST Webbook
$\Delta_{fus} H$	22.54	kJ/mol	377.7	NIST Webbook
$\Delta_{sub} H$	80.00 ± 0.50	kJ/mol	302.5	NIST Webbook
$\Delta_{sub} H$	81.00 ± 2.00	kJ/mol	309.0	NIST Webbook
$\Delta_{vap} H$	61.20	kJ/mol	408.5	NIST Webbook
$\Delta_{vap} H$	63.10	kJ/mol	457.0	NIST Webbook
$\Delta_{fus} S$	60.30	J/mol×K	337.5	NIST Webbook
$\Delta_{fus} S$	58.00	J/mol×K	376.85	NIST Webbook

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H6O2/c7-5-3-1-2-4-6\(5\)8/h1-4,7-8H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H6O2/c7-5-3-1-2-4-6(5)8/h1-4,7-8H)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$\Delta_c H^\circ_{\text{solid}}$ : Standard solid enthalpy of combustion (kJ/mol).  
 $C_{p,\text{gas}}$ : Ideal gas heat capacity (J/mol $\times$ K).  
 $C_{p,\text{solid}}$ : Solid phase heat capacity (J/mol $\times$ K).  
 $\eta$ : Dynamic viscosity (Pa $\times$ s).  
 $\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).  
 $\Delta_f H^\circ_{\text{gas}}$ : Enthalpy of formation at standard conditions (kJ/mol).  
 $\Delta_f H^\circ_{\text{solid}}$ : Solid phase enthalpy of formation at standard conditions (kJ/mol).  
 $\Delta_{\text{fus}} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).  
 $\Delta_{\text{fus}} H$ : Enthalpy of fusion at a given temperature (kJ/mol).  
 $\Delta_{\text{sub}} H^\circ$ : Enthalpy of sublimation at standard conditions (kJ/mol).  
 $\Delta_{\text{sub}} H$ : Enthalpy of sublimation at a given temperature (kJ/mol).  
 $\Delta_{\text{vap}} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).  
 $\Delta_{\text{vap}} H$ : Enthalpy of vaporization at a given temperature (kJ/mol).  
**IE**: Ionization energy (eV).  
**logP<sub>oct/wat</sub>**: Octanol/Water partition coefficient .  
 $P_c$ : Critical Pressure (kPa).  
 $\Delta_{\text{fus}} S$ : Entropy of fusion at a given temperature (J/mol $\times$ K).  
 $T_{\text{boil}}$ : Normal Boiling Point Temperature (K).  
 $T_c$ : Critical Temperature (K).  
 $T_{\text{fus}}$ : Normal melting (fusion) point (K).  
 $T_{\text{triple}}$ : Triple Point Temperature (K).  
 $V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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