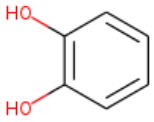
1,2-Benzenediol

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

Property	Value	Unit	Source
$\Delta_{sub}H°$	87.50 ± 0.29	kJ/mol	NIST Webbook
$\Delta_{sub}H°$	87.50	kJ/mol	NIST Webbook
$\Delta_{sub}H°$	87.50 ± 0.30	kJ/mol	NIST Webbook
$\Delta_{sub}H°$	86.60 ± 1.60	kJ/mol	NIST Webbook
$\Delta_{sub}H°$	86.60 ± 1.60	kJ/mol	NIST Webbook
$\Delta_{sub}H°$	86.60	kJ/mol	NIST Webbook
$\Delta_{sub}H°$	81.50	kJ/mol	NIST Webbook
$\Delta_{vap}H°$	71.90 ± 0.80	kJ/mol	NIST Webbook
IE	8.15	eV	NIST Webbook
IE	8.56	eV	NIST Webbook
$logP_{oct/wat}$	1.10		Crippen Method
P_c	7561.44	kPa	Joback Method
T_{boil}	518.20	K	NIST Webbook
T_{boil}	513.00	K	NIST Webbook
T_{boil}	518.80 ± 0.40	K	NIST Webbook
T_{boil}	519.05 ± 0.50	K	NIST Webbook
T_c	766.85	K	Joback Method
T_{fus}	376.90 ± 0.30	K	NIST Webbook
T_{fus}	377.70 ± 0.10	K	NIST Webbook
T_{fus}	378.00	K	NIST Webbook
T_{fus}	378.00 ± 1.00	K	NIST Webbook
T_{fus}	376.55 ± 0.50	K	NIST Webbook
T_{fus}	376.35 ± 0.50	K	NIST Webbook
T_{triple}	377.50 ± 0.20	K	NIST Webbook
V_c	0.20	m^3/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
η	0.00	Pa×s	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
NIST Webbook: 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/ci990307l

Legend

Δ_c**H°**$_{solid}$: Standard solid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
C$_{p,solid}$: Solid phase heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_f**H°**$_{solid}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{fus}**H**: Enthalpy of fusion at a given temperature (kJ/mol).
Δ_{sub}**H°**: Enthalpy of sublimation at standard conditions (kJ/mol).
Δ_{sub}**H**: Enthalpy of sublimation at a given temperature (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
Δ_{vap}**H**: Enthalpy of vaporization at a given temperature (kJ/mol).
IE: Ionization energy (eV).
***log*P**$_{oct/wat}$: Octanol/Water partition coefficient .
P$_c$: Critical Pressure (kPa).
Δ_{fus}**S**: Entropy of fusion at a given temperature (J/mol×K).
T$_{boil}$: Normal Boiling Point Temperature (K).
T$_c$: Critical Temperature (K).
T$_{fus}$: Normal melting (fusion) point (K).
T$_{triple}$: Triple Point Temperature (K).
V$_c$: Critical Volume (m^3/kg-mol).