

# 1,2,3-Benzenetriol

<b>Other names:</b>	1,2,3-TRIHYDROXYBENZENE 1,2,3-Trihydroxybenzen 2,3-Dihydroxyphenol Benzene, 1,2,3-trihydroxy- Benzene-1,2,3-triol C.I. 76515 C.I. 76551 C.I. Oxidation Base 32 Fouramine Brown AP Fouramine base ap Fourrine 85 Fourrine PG NSC 5035 PYROGALLOL Phenol Piral Pyro Pyrogallic acid
<b>Inchi:</b>	InChI=1S/C6H6O3/c7-4-2-1-3-5(8)6(4)9/h1-3,7-9H
<b>InchiKey:</b>	WQGWDDDVZFFDIG-UHFFFAOYSA-N
<b>Formula:</b>	C6H6O3
<b>SMILES:</b>	Oc1cccc(O)c1O
<b>Mol. weight [g/mol]:</b>	126.11
<b>CAS:</b>	87-66-1

## Physical Properties

Property code	Value	Unit	Source
chs	-2586.00	kJ/mol	NIST Webbook
chs	-2667.40 ± 0.50	kJ/mol	NIST Webbook
gf	-342.18	kJ/mol	Joback Method
hf	-434.20 ± 1.10	kJ/mol	NIST Webbook
hfs	-551.10 ± 0.90	kJ/mol	NIST Webbook
hfus	23.07	kJ/mol	Joback Method
hsub	104.00	kJ/mol	NIST Webbook
hsub	116.90 ± 0.60	kJ/mol	NIST Webbook
hsub	116.90	kJ/mol	NIST Webbook
hsub	116.90 ± 0.60	kJ/mol	NIST Webbook

hvap	69.61		kJ/mol	Joback Method
log10ws	-0.12			Crippen Method
logp	0.803			Crippen Method
mcvol	89.250		ml/mol	McGowan Method
pc	9980.03		kPa	Joback Method
rinpol	1329.00			NIST Webbook
rinpol	1341.00			NIST Webbook
rinpol	1329.00			NIST Webbook
rinpol	1385.70			NIST Webbook
rinpol	1329.00			NIST Webbook
tb	582.20		K	NIST Webbook
tb	582.15 ± 1.00		K	NIST Webbook
tc	858.52		K	Joback Method
tf	398.65 ± 0.50		K	NIST Webbook
tf	407.00 ± 1.00		K	NIST Webbook
vc	0.162		m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.40	J/molxK	600.24	Joback Method
cpg	229.07	J/molxK	643.29	Joback Method
cpg	235.05	J/molxK	686.33	Joback Method
cpg	240.59	J/molxK	729.38	Joback Method
cpg	245.92	J/molxK	772.43	Joback Method
cpg	251.30	J/molxK	815.47	Joback Method
cpg	256.97	J/molxK	858.52	Joback Method
dvisc	0.0000013	Paxs	600.24	Joback Method
dvisc	0.0000112	Paxs	522.07	Joback Method
dvisc	0.0000185	Paxs	506.44	Joback Method
dvisc	0.0000045	Paxs	553.34	Joback Method
dvisc	0.0000029	Paxs	568.97	Joback Method
dvisc	0.0000020	Paxs	584.61	Joback Method
dvisc	0.0000070	Paxs	537.71	Joback Method
hfust	25.90	kJ/mol	405.60	NIST Webbook
hfust	18.55	kJ/mol	407.20	NIST Webbook
hfust	18.55	kJ/mol	407.20	NIST Webbook
hsubt	89.10	kJ/mol	387.50	NIST Webbook
hvapt	69.50	kJ/mol	503.50	NIST Webbook

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	444.20	K	1.60	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.11663e+01
Coeff. B	-1.11494e+04
Coeff. C	9.16120e+01
Temperature range (K), min.	435.15
Temperature range (K), max.	611.61

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	-8.48206e+00
Coeff. B	-7.36523e+03
Coeff. C	4.17478e+00
Coeff. D	-2.41200e-06
Temperature range (K), min.	407.00
Temperature range (K), max.	830.00

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>KDB:</b>	<a href="https://www.cheric.org/files/research/kdb/mol/mol866.mol">https://www.cheric.org/files/research/kdb/mol/mol866.mol</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C87661&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C87661&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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