1,2,3-Benzenetriol

Other names:	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
Inchi:	InChI=1S/C6H6O3/c7-4-2-1-3-5(8)6(4)9/h1-3,7-9H
InchiKey:	WQGWDDDVZFFDIG-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	Oc1cccc(O)c1O
Mol. weight [g/mol]:	126.11
CAS:	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	116.90 ± 0.60	kJ/mol	NIST Webbook
hsub	116.90	kJ/mol	NIST Webbook
hsub	104.00	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	1385.70		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1329.00		NIST Webbook
tb	582.15 ± 1.00	K	NIST Webbook
tb	582.20	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.07	J/mol×K	643.29	Joback Method
cpg	235.05	J/mol×K	686.33	Joback Method
cpg	240.59	J/mol×K	729.38	Joback Method
cpg	256.97	J/mol×K	858.52	Joback Method
cpg	245.92	J/mol×K	772.43	Joback Method
cpg	251.30	J/mol×K	815.47	Joback Method
cpg	222.40	J/mol×K	600.24	Joback Method
dvisc	0.0000020	Pa×s	584.61	Joback Method
dvisc	0.0000029	Pa×s	568.97	Joback Method
dvisc	0.0000045	Pa×s	553.34	Joback Method
dvisc	0.0000070	Pa×s	537.71	Joback Method
dvisc	0.0000112	Pa×s	522.07	Joback Method
dvisc	0.0000013	Pa×s	600.24	Joback Method
dvisc	0.0000185	Pa×s	506.44	Joback Method
hfust	18.55	kJ/mol	407.20	NIST Webbook
hfust	25.90	kJ/mol	405.60	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(Pvp) = 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(Pvp) = A + B/T + C*ln(T) + D*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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol866.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C87661&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=866

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume