2,3-Butanediol

Other names:	2,3-BUTYLENE GLYCOL
	2,3-Butandiol
	2,3-Butanediol, isomer 1
	2,3-Butanediol, isomer 2
	2,3-Dihydroxybutane
	2,3-butanediol, isomer not specified
	2,3-butanodiol
	2,3-butyleneglycol
	2,3-butyleneglycol, isomer not specified
	2.3-Butanediol, isomer 3
	Butane-2,3-diol
	D-2,3-Butane diol
	DIMETHYLETHYLENE GLYCOL
	butane, 2,3-dihydroxy-, isomer not specified
Inchi:	InChI=1S/C4H10O2/c1-3(5)4(2)6/h3-6H,1-2H3
InchiKey:	OWBTYPJTUOEWEK-UHFFFAOYSA-N
Formula:	C4H10O2
SMILES:	CC(O)C(C)O
Mol. weight [g/mol]:	90.12
CAS:	513-85-9

Physical Properties

Property code	Value	Unit	Source
chl	-2461.00	kJ/mol	NIST Webbook
cpl	236.63	J/mol×K	Molar heat capacities for {isomer of butanediol + methanol} as function of mixture composition and temperature
gf	-295.72	kJ/mol	Joback Method
hf	-440.91	kJ/mol	Joback Method
hfl	-544.80	kJ/mol	NIST Webbook
hfl	-541.80	kJ/mol	NIST Webbook
hfus	7.25	kJ/mol	Joback Method
hvap	57.08	kJ/mol	Joback Method
log10ws	-0.25		Crippen Method
logp	-0.252		Crippen Method
mcvol	78.960	ml/mol	McGowan Method

pc	5087.49	kPa	Joback Method
rinpol	767.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	747.50		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	802.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1539.00		NIST Webbook

ripol	1521.00	NIST Webbook
ripol	1541.00	NIST Webbook
ripol	1558.00	NIST Webbook
ripol	1554.00	NIST Webbook
ripol	1566.00	NIST Webbook
ripol	1512.00	NIST Webbook
ripol	1494.00	NIST Webbook
ripol	1494.00	NIST Webbook
ripol	1492.00	NIST Webbook
ripol	1492.00	NIST Webbook
ripol	1522.00	NIST Webbook
ripol	1526.00	NIST Webbook
ripol	1580.00	NIST Webbook
ripol	1545.00	NIST Webbook
ripol	1570.00	NIST Webbook
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ripol	1579.00	NIST Webbook
ripol	1558.00	NIST Webbook
ripol	1562.00	NIST Webbook
ripol	1522.00	NIST Webbook
ripol	1541.00	NIST Webbook
ripol	1576.00	NIST Webbook
ripol	1554.00	NIST Webbook
ripol	1580.00	NIST Webbook
ripol	1542.00	NIST Webbook
ripol	1558.00	NIST Webbook
ripol	1523.00	NIST Webbook
ripol	1566.00	NIST Webbook
ripol	1539.00	NIST Webbook
ripol	1539.00	NIST Webbook
ripol	1526.00	NIST Webbook
ripol	1517.00	NIST Webbook
ripol	1512.00	NIST Webbook
ripol	1529.00	NIST Webbook

ripol	1536.00		NIST Webbook
ripol	1590.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1583.00		NIST Webbook
tb	454.21	K	Liquid liquid equilibria of water + 2,3-butanediol + ethyl acetate at several temperatures
tb	454.21	K	Liquid liquid equilibria of water + 2,3-butanediol + 1-butanol at T = 298.15 K, T = 308.15K and T = 318.15K
tb	415.15 ± 3.00	K	NIST Webbook
tb	455.15 ± 4.00	K	NIST Webbook
tb	455.65 ± 1.00	K	NIST Webbook
tb	454.21	K	Liquid Liquid Equilibria of Water + 2,3-Butanediol + Butyl Acetate at T) 298.15 K, T) 308.15 K, and T) 318.15 K
tb	454.21	K	Vapor liquid equilibria for the binary mixtures of 2,3-butanediol with n-butanol, n-butyl acetate, and ethyl acetate at 101.3 kPa
tb	456.70	K	NIST Webbook
tc	639.26	K	Joback Method
tf	292.15 ± 2.00	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.21	J/mol×K	556.83	Joback Method
cpg	180.37	J/mol×K	501.88	Joback Method
cpg	173.55	J/mol×K	474.40	Joback Method
cpg	199.24	J/mol×K	584.30	Joback Method
cpg	205.02	J/mol×K	611.78	Joback Method

cpg	210.57	J/mol×K	639.26	Joback Method
cpg	186.92	J/mol×K	529.35	Joback Method
cpl	249.23	J/mol×K	323.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	246.82	J/mol×K	318.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	251.60	J/mol×K	328.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	241.85	J/mol×K	308.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	239.28	J/mol×K	303.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	236.67	J/mol×K	298.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature

cpl	253.91	J/mol×K	333.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	256.17	J/mol×K	338.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	258.39	J/mol×K	343.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	260.55	J/mol×K	348.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	262.67	J/mol×K	353.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	244.35	J/mol×K	313.15	Molar heat capacities for (1-butanol + 1,4-butanediol, 2,3-butanediol, 1,2-butanediol, and 2-methyl-2,4-pentanediol) as function of temperature
cpl	213.00	J/mol×K	298.20	NIST Webbook
dvisc	0.0002812	Pa×s	433.08	Joback Method
dvisc	0.1120965	Pa×s	267.80	Joback Method

dvisc	0.0137635	Pa×s	309.12	Joback Method
dvisc	0.0027712	Pa×s	350.44	Joback Method
dvisc	0.0007824	Pa×s	391.76	Joback Method
dvisc	1.9625358	Pa×s	226.48	Joback Method
dvisc	0.0001208	Pa×s	474.40	Joback Method
hvapt	55.70	kJ/mol	379.50	NIST Webbook
hvapt	57.90	kJ/mol	378.00	NIST Webbook
hvapt	58.40	kJ/mol	386.00	NIST Webbook
hvapt	62.50	kJ/mol	402.50	NIST Webbook
rfi	1.43660		298.15	Densities, Dynamic Viscosities, Speeds of Sound, and Relative Permittivities for Water + Alkanediols (Propane-1,2- and -1,3-diol and Butane-1,2-, -1,3-, -1,4-, and -2,3-Diol) at Different Temperatures
rhol	990.72	kg/m3	308.15	Effect of placement of hydroxyl groups in isomeric butanediol on the behaviour of thermophysical and spectroscopic properties of pyrrolidin-2-one
rhol	990.72	kg/m3	308.15	A comparative study of thermophysical and spectroscopic properties in mixtures of isomeric butanediol and N,N-dimethylformamide
rhol	990.72	kg/m3	308.15	Thermodynamic, transport, and spectroscopic studies for mixtures of isomeric butanediol and N-methyl-2-pyrrolidinone

rhol	990.72	kg/m3	308.15	Effect of B-cyclodextrin on the behaviour of thermophysical and spectroscopic properties of binary mixtures of (isomeric butanediol + pyrrolidin-2-one)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62445e+01
Coeff. B	-4.52281e+03
Coeff. C	-6.76820e+01
Temperature range (K), min.	351.12
Temperature range (K), max.	481.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.37891e+02
Coeff. B	-1.22864e+04
Coeff. C	-1.78282e+01
Coeff. D	1.38579e-05
Temperature range (K), min.	280.75
Temperature range (K), max.	611.00

Sources

Effect of hydrophilic additives on volumetric and viscosity properties of amino acids in aqueous solutions at T = (283.15 to 298.15) K:	https://www.doi.org/10.1016/j.jct.2011.12.020
Effect of placement of hydroxyl groups in isomeric butanediol on the behavior of thermophysical and spectroscopic properties of pyrrolidin-2-one:	https://www.doi.org/10.1016/j.jct.2004.11.020
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=918
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=918
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Densities, partial molar volumes at infinite dilution, side chain partial molar volumes and transfer volumes of dipeptides in sucrose and 2,3-butanediol aqueous solutions at T = (283.15 - 333.15) K:	https://www.doi.org/10.1021/je100703r

A comparative study of thermophysical and spectroscopic properties in mixtures of isomeric butanediol and N-methyl-2-pyrrolidinone:	https://www.doi.org/10.1016/j.jct.2005.09.001
Solubilities of Carbon Dioxide in Eutectic Mixtures of Choline Chloride and Dihydric Alcohols:	https://www.doi.org/10.1021/je400884v
Vapor-liquid equilibria for the binary mixtures of 2,3-butanediol with n-butanol, n-butyl acetate, and ethyl acetate at 101.3 kPa:	https://www.doi.org/10.1016/j.fluid.2007.09.001
Effect of β-cyclodextrin on the behaviour of thermophysical and spectroscopic properties of binary mixtures of isomeric butanediol + pyrrolidin-2-one):	https://www.doi.org/10.1016/j.jct.2012.08.026
Liquid-phase behavior of hexafluorophosphate ionic liquids with 2-butanol:	https://www.doi.org/10.1016/j.fluid.2011.11.004
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C513859&Units=SI
Liquid liquid equilibria of water + 2,3-butanediol + ethyl acetate at several temperatures:	https://www.doi.org/10.1016/j.fluid.2008.01.009
Liquid-liquid equilibria of water + 2,3-butanediol + isobutanol at several temperatures:	https://www.doi.org/10.1016/j.fluid.2012.04.018
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid Liquid Equilibria for the Ternary Systems of Water + Butane-2,3-diol + 2-Methylbutan-1-ol, 2-Ethylbutan-1-ol, and 4-Methylpentan-2-ol at 298.15 and 308.15 K:	https://www.doi.org/10.1021/acs.jced.6b00945
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Phase behavior of imidazolium and phosphonium tetrafluoroborates with dihydroxy alcohols:	https://www.doi.org/10.1016/j.fluid.2014.08.028
Isopiestic determination of osmotic and activity coefficients of aqueous solutions of aliphatic polyols at 298.2 K:	https://www.doi.org/10.1016/j.fluid.2005.12.016
Thermodynamics and activity coefficients at infinite dilution for organic solutes, water and ions in the ionic liquid choline bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2014.04.024
Crippen Method:	https://www.doi.org/10.1016/j.jct.2009.11.018
Experimental study of the excess molar volume of ternary mixtures containing 1,3-propanediol, or 1,2-butanediol, or 1,3-butanediol, or 1,4-butanediol, or 2,3-butanediol + water + alcohol at temperature of 298.15 K and atmospheric pressure:	https://www.chemeo.com/doc/models/crippen_log10ws
Osmotic coefficient data and an excess Gibbs energy function for single-phase aqueous solutions of glycols + alcohol mixtures at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2008.11.016
Densities, Dynamic Viscosities, Speeds of Sound, and Relative Permittivities for Water + Alkanediols (Propane-1,2- and -1,3-diol and Butane-1,2-, -1,3-, -1,4-, and -2,3-diol) at Different Temperatures:	https://www.doi.org/10.1021/je0340755
Liquid-liquid phase equilibria for (water + 2,3-butanediol + 1-alcohol) ternary systems at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2007.04.011
Liquid-liquid equilibria of (1-butanol + 2,3-butanediol + water) at different temperatures:	https://www.doi.org/10.1016/j.jct.2008.10.004
Liquid-liquid equilibria of water + 2,3-butanediol + 1-butanol at T = 298.15 K, T = 308.15K and T = 318.15K:	https://www.doi.org/10.1016/j.fluid.2007.12.003
Molar heat capacities for isomer of butanediol + methanol} as function of mixture composition and temperature:	https://www.doi.org/10.1016/j.jct.2014.07.023
Enthalpies of dilution of aqueous solutions of n-butanol, butanediols, 1,2,4-butanetriol, and 2,2,2,4-butanetetrol at 298.15K:	https://www.doi.org/10.1016/j.tca.2005.06.014
Liquid Liquid Equilibria of Water + 2,3-Butanediol + Butyl Acetate at T) 298.15 K, T) 308.15 K, and T) 318.15 K:	https://www.doi.org/10.1021/je700705d
Liquid-liquid equilibria of water + 2,3-butanediol + 2-ethyl-1-hexanol) at several temperatures:	https://www.doi.org/10.1016/j.fluid.2006.06.025
Thermodynamic, transport, and spectroscopic studies for mixtures of isomeric butanediol and N-methyl-2-pyrrolidinone:	https://www.doi.org/10.1016/j.jct.2009.06.006

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume