2-Butanol, 3-methyl-

Other names:	(.+/-.)-3-Methyl-2-butanol
	(CH3)2CHCH(OH)CH3
	1,2-Dimethyl-1-propanol
	1,2-Dimethylpropanol
	2-Methyl-3-butanol
	3-METHYL-2-BUTANOL
	3-Methyl-butan-2-ol
	Butan-2-ol, 3-methyl-
	METHYLISOPROPYLCARBINOL
	NSC 71162
	SEC-ISOAMYL ALCOHOL
Inchi:	InChI=1S/C5H12O/c1-4(2)5(3)6/h4-6H,1-3H3
InchiKey:	MXLMTQWGSQIYOW-UHFFFAOYSA-N
Formula:	C5H12O
SMILES:	CC(C)C(C)O
Mol. weight [g/mol]:	88.15
CAS:	598-75-4

Physical Properties

Property code	Value	Unit	Source
chl	-3315.10 ± 0.63	kJ/mol	NIST Webbook
gf	-150.48	kJ/mol	Joback Method
hf	-313.10	kJ/mol	NIST Webbook
hf	-316.40 ± 1.80	kJ/mol	NIST Webbook
hfl	-369.90 ± 1.40	kJ/mol	NIST Webbook
hfl	-366.60 ± 0.71	kJ/mol	NIST Webbook
hfus	5.75	kJ/mol	Joback Method
hvap	51.70	kJ/mol	NIST Webbook
hvap	53.50 ± 0.40	kJ/mol	NIST Webbook
hvap	51.60 ± 0.30	kJ/mol	NIST Webbook
hvap	53.03	kJ/mol	NIST Webbook
ie	9.75 ± 0.05	eV	NIST Webbook
ie	10.01 ± 0.07	eV	NIST Webbook
log10ws	-0.20		Aqueous Solubility Prediction Method
log10ws	-0.18		Estimated Solubility Method

logp	1.023		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3870.00 ± 20.00	kPa	NIST Webbook
pc	3870.00 ± 40.00	kPa	NIST Webbook
pc	3870.00	kPa	KDB
rinpol	666.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	692.10		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	670.00		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	692.10		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	663.00		NIST Webbook
ripol	1118.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1091.00		NIST Webbook

ripol	1089.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1124.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1108.00		NIST Webbook
sg	388.60 ± 3.80	J/mol×K	NIST Webbook
tb	386.15 ± 2.00	K	NIST Webbook
tb	386.55 ± 0.70	K	NIST Webbook
tb	386.05 ± 1.00	K	NIST Webbook
tb	387.15 ± 1.00	K	NIST Webbook
tb	381.15 ± 3.00	K	NIST Webbook
tb	383.90 ± 1.50	K	NIST Webbook
tb	385.20 ± 1.00	K	NIST Webbook
tb	384.55 ± 0.50	K	NIST Webbook
tb	384.65 ± 2.00	K	NIST Webbook
tb	385.15 ± 1.50	K	NIST Webbook
tb	386.15 ± 3.00	K	NIST Webbook
tb	386.05 ± 0.50	K	NIST Webbook
tb	386.65 ± 1.00	K	NIST Webbook
tb	385.00 ± 1.00	K	NIST Webbook
tb	384.95 ± 0.50	K	NIST Webbook
tb	384.65 ± 1.00	K	NIST Webbook
tb	386.65 ± 2.00	K	NIST Webbook
tb	388.15 ± 2.00	K	NIST Webbook
tb	382.15 ± 2.00	K	NIST Webbook
tb	383.15 ± 2.00	K	NIST Webbook
tb	385.20	K	NIST Webbook
tb	383.20 ± 2.00	K	NIST Webbook
tb	385.55 ± 1.00	K	NIST Webbook
tc	556.10 ± 0.50	K	NIST Webbook
tc	556.10	K	KDB
tc	556.10 ± 0.70	K	NIST Webbook
tf	176.93	K	Joback Method
tt	131.50 ± 0.70	K	NIST Webbook
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.84	J/mol×K	405.10	Joback Method
cpg	178.73	J/mol×K	433.25	Joback Method
cpg	187.29	J/mol×K	461.41	Joback Method
cpg	195.52	J/mol×K	489.56	Joback Method
cpg	203.43	J/mol×K	517.72	Joback Method
cpg	211.03	J/mol×K	545.87	Joback Method
cpg	218.33	J/mol×K	574.03	Joback Method
cpl	245.90	J/mol×K	298.15	NIST Webbook
cps	83.46	J/mol×K	110.42	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	69.50	J/mol×K	92.44	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	70.82	J/mol×K	93.66	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	70.42	J/mol×K	94.37	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	72.69	J/mol×K	95.60	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	72.33	J/mol×K	96.30	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	73.76	J/mol×K	97.54	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols

cps	73.35	J/mol×K	98.24	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	75.44	J/mol×K	99.48	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	75.01	J/mol×K	100.17	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	76.81	J/mol×K	101.42	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	76.45	J/mol×K	102.11	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	78.23	J/mol×K	103.37	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	77.94	J/mol×K	104.06	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	79.77	J/mol×K	105.32	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	79.31	J/mol×K	106.00	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	80.89	J/mol×K	107.95	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols

cps	82.57	J/mol×K	109.90	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	69.65	J/mol×K	91.72	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	82.24	J/mol×K	110.85	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	84.29	J/mol×K	111.85	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	84.44	J/mol×K	112.07	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	85.97	J/mol×K	113.80	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	86.22	J/mol×K	114.04	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	87.69	J/mol×K	115.76	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	87.96	J/mol×K	116.00	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	89.53	J/mol×K	117.71	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	

cps	91.40	J/mol×K	119.67	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	93.27	J/mol×K	121.44	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	93.55	J/mol×K	121.62	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	94.36	J/mol×K	122.07	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	95.77	J/mol×K	123.27	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	95.92	J/mol×K	123.58	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	98.99	J/mol×K	125.24	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	98.88	J/mol×K	125.53	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	102.70	J/mol×K	127.20	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	
cps	103.22	J/mol×K	127.49	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols	

cps	107.45	J/mol×K	129.14	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	68.52	J/mol×K	90.50	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	66.46	J/mol×K	88.57	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	66.12	J/mol×K	88.50	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	65.91	J/mol×K	87.96	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	65.12	J/mol×K	86.61	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	64.92	J/mol×K	85.35	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	68.19	J/mol×K	89.76	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
cps	64.32	J/mol×K	84.80	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
dvisc	0.9991270	Pa×s	176.93	Joback Method
dvisc	0.0759974	Pa×s	214.96	Joback Method
dvisc	0.0033141	Pa×s	291.01	Joback Method
dvisc	0.0011912	Pa×s	329.04	Joback Method
dvisc	0.0005293	Pa×s	367.07	Joback Method
dvisc	0.0002739	Pa×s	405.10	Joback Method

dvisc	0.0125411	Pa×s	252.99	Joback Method
hvapt	52.70	kJ/mol	341.00	NIST Webbook
hvapt	49.00	kJ/mol	327.50	NIST Webbook
hvapt	46.40	kJ/mol	339.00	NIST Webbook
pvap	81.33	kPa	378.81	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	61.33	kPa	371.24	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	65.33	kPa	372.90	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	70.66	kPa	374.99	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	75.99	kPa	376.95	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	53.33	kPa	367.65	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	86.66	kPa	380.58	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	91.99	kPa	382.26	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	97.33	kPa	383.87	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	99.33	kPa	384.45	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	49.33	kPa	365.69	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2

pvap	45.33	kPa	363.60	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	42.00	kPa	361.74	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	38.66	kPa	359.76	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	35.33	kPa	357.63	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	32.00	kPa	355.33	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	28.66	kPa	352.84	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	57.33	kPa	369.50	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
rfi	1.40700		298.15	Vapor-Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Methylpentane, 3-Methyl-2-butanone and 3-Methyl-2-butanol
rhol	804.35	kg/m3	308.15	Excess molar enthalpies of the binary systems: (Dibutyl ether + isomers of pentanol) at T = (298.15 and 308.15) K
rhol	813.09	kg/m3	298.15	Excess molar enthalpies of the binary systems: (Dibutyl ether + isomers of pentanol) at T = (298.15 and 308.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40003e+01
Coeff. B	-2.53974e+03
Coeff. C	-1.14297e+02
Temperature range (K), min.	299.51
Temperature range (K), max.	406.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.03416e+02
Coeff. B	-1.39925e+04
Coeff. C	-2.76617e+01
Coeff. D	1.51147e-05
Temperature range (K), min.	188.00
Temperature range (K), max.	574.00

Sources

Excess molar enthalpies of the binary systems: (Dibutyl ether + isomers of pentanol) at T = (298.15 and 308.15) K:	https://www.doi.org/10.1016/j.jct.2015.03.021
KDB Pure (Key Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=831
Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2 :	https://www.doi.org/10.1016/j.fluid.2010.06.020
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Measurement and modeling of high-pressure (vapor + liquid) equilibria of (CO2 + alkanol) binary systems:	https://www.doi.org/10.1016/j.jct.2010.12.018
Grigoras Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=831
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598754&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols:	https://www.doi.org/10.1021/je060411g
Temperature Dependence of Limiting Activity Coefficients, Henry s Law Constants, and Related Infinite Dilution	https://www.doi.org/10.1021/je901063s
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Properties of Branched Pentanols in Water: Measurement, Critical Compilation, Correlation, and Recommended Data:	https://www.doi.org/10.1021/je050062a
Vapor−Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Methylpentane, 3-Methyl-2-butanone and 3-Methyl-2-butanol:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=831
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid 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
ie:	Ionization energy
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
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume