2-Butanol

Other names:	1-Methyl propanol
	1-Methyl-1-propanol
	1-Methylpropyl alcohol
	2-Butyl alcohol
	2-Hydroxybutane
	Alcool butylique secondaire
	Butan-2-ol
	Butane, 2-hydroxy-
	Butanol secondaire
	Butanol-2
	Butylene hydrate
	CCS 301
	DL-2-Butanol
	DL-sec-Butanol
	Ethyl methyl carbinol
	METHYLETHYLCARBINOL
	Methyl ethyl carbinol
	NSC 25499
	SEC-BUTANOL
	SEC-BUTYL ALCOHOL
	n-Butan-2-ol
	s-Butanol
	s-Butyl alcohol
	sec-C4H9OH
Inchi:	InChI=1S/C4H10O/c1-3-4(2)5/h4-5H,3H2,1-2H3
InchiKey:	BTANRVKWQNVYAZ-UHFFFAOYSA-N
Formula:	C4H10O
SMILES:	CCC(C)O
Mol. weight [g/mol]:	74.12
CAS:	78-92-2

Physical Properties

Property code	Value	Unit	Source
af	0.5770		KDB
affp	815.00	kJ/mol	NIST Webbook
aigt	679.26	K	KDB

basg	784.60	kJ/mol	NIST Webbook
chl	-2660.60 ± 0.92	kJ/mol	NIST Webbook
chl	-2660.60 ± 0.54	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
fll	1.70	% in Air	KDB
flu	9.00	% in Air	KDB
fpo	297.04	K	KDB
gf	-167.70	kJ/mol	KDB
gyrad	3.1820		KDB
hf	-293.00 ± 1.50	kJ/mol	NIST Webbook
hf	-292.80	kJ/mol	KDB
hf	-293.10	kJ/mol	NIST Webbook
hfl	-342.70 ± 0.59	kJ/mol	NIST Webbook
hfl	-342.60 ± 0.92	kJ/mol	NIST Webbook
hfus	6.68	kJ/mol	Joback Method
hvap	40.79	kJ/mol	Joback Method
ie	10.35 ± 0.03	eV	NIST Webbook
ie	10.23	eV	NIST Webbook
ie	9.88	eV	NIST Webbook
ie	9.88	eV	NIST Webbook
ie	9.88 ± 0.07	eV	NIST Webbook
ie	9.88 ± 0.03	eV	NIST Webbook
ie	9.88 ± 0.03	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	0.777		Crippen Method
mcvol	73.090	ml/mol	McGowan Method
pc	4202.00	kPa	KDB
rhoc	275.73 ± 1.48	kg/m3	NIST Webbook
rhoc	275.51	kg/m3	NIST Webbook
rhoc	275.73	kg/m3	NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	563.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	600.60		NIST Webbook
rinpol	602.20		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	603.00		NIST Webbook

rinpol	586.00	NIST Webbook
rinpol	565.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	585.00	NIST Webbook
rinpol	594.00	NIST Webbook
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ripol	1019.00	NIST Webbook
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ripol	1000.00	NIST Webbook
ripol	1005.00	NIST Webbook
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ripol	1013.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	1001.00		NIST Webbook
sg	355.37	J/mol×K	NIST Webbook
sl	214.70	J/mol×K	NIST Webbook
sl	213.10	J/mol×K	NIST Webbook
tb	372.66	K	KDB
tc	536.10 ± 0.60	K	NIST Webbook
tc	536.20 ± 0.30	K	NIST Webbook
tc	536.20	K	KDB
tc	536.60	K	NIST Webbook
tc	536.10 ± 0.60	K	NIST Webbook
tc	538.30	K	NIST Webbook
tc	535.98	K	NIST Webbook
tc	536.00	K	NIST Webbook
tc	536.18	K	NIST Webbook
tf	158.45	K	NIST Webbook
tf	158.40	K	KDB
tt	184.73 ± 0.10	K	NIST Webbook
tt	184.70 ± 0.02	K	NIST Webbook
vc	0.269	m3/kmol	NIST Webbook
vc	0.269	m3/kmol	KDB

zc	0.2535390	KDB
zra	0.26	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.31 ± 0.67	J/mol×K	515.95	NIST Webbook
cpg	184.89 ± 0.67	J/mol×K	582.85	NIST Webbook
cpg	158.81 ± 0.67	J/mol×K	470.85	NIST Webbook
cpg	131.71 ± 0.40	J/mol×K	365.15	NIST Webbook
cpg	137.87 ± 0.67	J/mol×K	380.95	NIST Webbook
cpg	136.52 ± 0.41	J/mol×K	383.15	NIST Webbook
cpg	139.10 ± 0.67	J/mol×K	386.25	NIST Webbook
cpg	140.85 ± 0.67	J/mol×K	393.75	NIST Webbook
cpg	141.46 ± 0.42	J/mol×K	401.15	NIST Webbook
cpg	143.50 ± 0.67	J/mol×K	405.15	NIST Webbook
cpg	143.74 ± 0.67	J/mol×K	406.15	NIST Webbook
cpg	146.32 ± 0.67	J/mol×K	417.25	NIST Webbook
cpg	146.23 ± 0.44	J/mol×K	419.15	NIST Webbook
cpg	150.96 ± 0.45	J/mol×K	437.15	NIST Webbook
cpg	151.79 ± 0.67	J/mol×K	440.75	NIST Webbook
cpg	155.64 ± 0.47	J/mol×K	455.15	NIST Webbook
cpg	179.65 ± 0.67	J/mol×K	560.35	NIST Webbook
cpl	197.40	J/mol×K	298.15	NIST Webbook
cpl	196.80	J/mol×K	298.15	NIST Webbook
cpl	184.90	J/mol×K	281.70	NIST Webbook
cpl	197.10	J/mol×K	298.15	NIST Webbook
cpl	198.03	J/mol×K	298.15	NIST Webbook
cpl	196.67	J/mol×K	298.15	NIST Webbook
cpl	199.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0032653	Pa×s	281.66	Joback Method
dvisc	0.0012927	Pa×s	315.33	Joback Method
dvisc	0.0003304	Pa×s	382.66	Joback Method
dvisc	0.4179525	Pa×s	180.66	Joback Method
dvisc	0.0498950	Pa×s	214.33	Joback Method
dvisc	0.0106075	Pa×s	247.99	Joback Method
dvisc	0.0006119	Pa×s	348.99	Joback Method
hfust	5.97	kJ/mol	184.70	NIST Webbook
hfust	5.97	kJ/mol	184.70	NIST Webbook
hfust	5.97	kJ/mol	184.70	NIST Webbook
hfust	6.00	kJ/mol	177.38	NIST Webbook

hvapt	43.30 ± 0.10	kJ/mol	355.00	NIST Webbook
hvapt	41.90 ± 0.10	kJ/mol	365.00	NIST Webbook
hvapt	40.80 ± 0.10	kJ/mol	372.00	NIST Webbook
hvapt	40.79	kJ/mol	372.80	KDB
hvapt	40.75	kJ/mol	372.70	NIST Webbook
hvapt	48.80	kJ/mol	343.00	NIST Webbook
hvapt	46.20	kJ/mol	349.50	NIST Webbook
hvapt	47.70	kJ/mol	339.50	NIST Webbook
hvapt	49.30	kJ/mol	353.00	NIST Webbook
hvapt	43.20	kJ/mol	370.00	NIST Webbook
hvapt	47.90	kJ/mol	448.00	NIST Webbook
hvapt	57.50	kJ/mol	256.50	NIST Webbook
hvapt	43.20	kJ/mol	369.50	NIST Webbook
hvapt	42.00	kJ/mol	386.00	NIST Webbook
hvapt	39.60	kJ/mol	440.00	NIST Webbook
hvapt	35.00	kJ/mol	506.00	NIST Webbook
hvapt	44.70	kJ/mol	359.50	NIST Webbook
hvapt	47.80	kJ/mol	340.00	NIST Webbook
hvapt	53.20	kJ/mol	336.50	NIST Webbook
hvapt	44.10	kJ/mol	345.50	NIST Webbook
hvapt	50.20	kJ/mol	297.00	NIST Webbook
hvapt	48.10	kJ/mol	345.50	NIST Webbook
hvapt	46.30	kJ/mol	348.00	NIST Webbook
hvapt	44.10	kJ/mol	363.00	NIST Webbook
hvapt	45.30 ± 0.10	kJ/mol	340.00	NIST Webbook
rhol	807.00	kg/m3	293.00	KDB
sfust	32.32	J/mol×K	184.70	NIST Webbook
sfust	33.83	J/mol×K	177.38	NIST Webbook
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.03633e+02
Coeff. B	-9.51804e+03
Coeff. C	-1.24851e+01
Coeff. D	3.34249e-06
Temperature range (K), min.	158.45
Temperature range (K), max.	536.01

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=823
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78922&Units=SI
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=823
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=823
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter

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