1-Butanol, 2-ethyl-

Other names:	2-Ethyl-1-butanol
	2-Ethylbutan-1-ol
	2-Ethylbutanol
	2-Ethylbutanol-1
	2-Ethylbutyl alcohol
	3-METHYLOLPENTANE
	3-Pentyl carbinol
	NSC 8858
	PSEUDOHEXYL ALCOHOL
	UN 2275
Inchi:	InChI=1S/C6H14O/c1-3-6(4-2)5-7/h6-7H,3-5H2,1-2H3
InchiKey:	TZYRSLHNPKPEFV-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCC(CC)CO
Mol. weight [g/mol]:	102.17
CAS:	97-95-0

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-324.68	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	60.30 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.17		Estimated Solubility Method
log10ws	-1.17		Aqueous Solubility Prediction Method
logp	1.415		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
pc	3484.76	kPa	Joback Method
rinpol	834.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	819.00		NIST Webbook

rinpol	834.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	806.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1318.00		NIST Webbook
tb	423.15 ± 3.00	K	NIST Webbook
tb	418.65 ± 2.00	K	NIST Webbook
tb	419.50	K	NIST Webbook
tb	420.15 ± 2.00	K	NIST Webbook
tb	420.45 ± 2.00	K	NIST Webbook
tb	418.15 ± 3.00	K	NIST Webbook
tb	421.15 ± 0.50	K	NIST Webbook
tb	422.15 ± 2.00	K	NIST Webbook
tb	419.45 ± 1.50	K	NIST Webbook
tb	420.65 ± 2.00	K	NIST Webbook
tb	421.65 ± 2.00	K	NIST Webbook
tb	422.10 ± 1.00	K	NIST Webbook
tb	420.15	K	NIST Webbook
tc	592.97	K	Joback Method
tf	158.75	K	NIST Webbook
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.25	J/mol×K	592.97	Joback Method

cpg	244.78	J/mol×K	538.12	Joback Method
cpg	253.18	J/mol×K	565.55	Joback Method
cpg	207.74	J/mol×K	428.42	Joback Method
cpg	217.54	J/mol×K	455.85	Joback Method
cpg	226.97	J/mol×K	483.27	Joback Method
cpg	236.05	J/mol×K	510.70	Joback Method
cpl	252.82	J/mol×K	298.15	NIST Webbook
cpl	246.65	J/mol×K	298.15	NIST Webbook
dvisc	0.0002400	Pa×s	428.42	Joback Method
dvisc	0.0008856	Pa×s	353.35	Joback Method
dvisc	0.0004330	Pa×s	390.88	Joback Method
dvisc	0.2179366	Pa×s	203.20	Joback Method
dvisc	0.0289027	Pa×s	240.74	Joback Method
dvisc	0.0066108	Pa×s	278.27	Joback Method
dvisc	0.0021472	Pa×s	315.81	Joback Method
hvapt	59.60	kJ/mol	362.00	NIST Webbook
hvapt	65.40	kJ/mol	278.50	NIST Webbook
hvapt	53.10	kJ/mol	373.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50939e+01
Coeff. B	-3.41499e+03
Coeff. C	-9.50050e+01
Temperature range (K), min.	325.65
Temperature range (K), max.	444.10

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.30270e+02
Coeff. B	-1.97516e+04
Coeff. C	-4.71831e+01
Coeff. D	3.61872e-05
Temperature range (K), min.	250.00
Temperature range (K), max.	580.00

Datasets

Speed of sound, m/s

Pressure, kPa - Liquid	Temperature, K - Liquid	Speed of sound, m/s - Liquid
101.00	292.89	1321.71
15200.00	292.86	1403.2
30390.00	292.85	1472.37
45590.00	292.85	1534.86
60790.00	292.85	1592.44
75990.00	292.84	1645.88
91180.00	292.85	1695.72
101320.00	292.85	1727.57
101.00	308.11	1265.89
15200.00	308.10	1351.8
30390.00	308.11	1424.12
45590.00	308.11	1489.3
60790.00	308.11	1549.01
75990.00	308.11	1604.28
91180.00	308.11	1655.77
101320.00	308.11	1688.13
101.00	298.15	1302.28
15200.00	298.15	1385.09
30390.00	298.15	1455.32
45590.00	298.15	1518.76
60790.00	298.15	1577.16
75990.00	298.15	1631.16
91180.00	298.15	1681.56
101320.00	298.15	1713.55
101.00	313.08	1247.84
15200.00	313.08	1335.35
30390.00	313.08	1409.02
45590.00	313.08	1474.98
60790.00	313.08	1535.15
75990.00	313.08	1591.18
91180.00	313.08	1643.09
101320.00	313.09	1675.87
101.00	303.13	1284.05

15200.00	303.12	1368.36
30390.00	303.11	1439.59
45590.00	303.11	1503.98
60790.00	303.11	1562.96
75990.00	303.12	1617.74
91180.00	303.12	1668.49
101320.00	303.11	1700.72
101.00	318.16	1229.47
15200.00	318.15	1318.79
30390.00	318.25	1393.2
45590.00	318.25	1460.26
60790.00	318.25	1521.19
75990.00	318.25	1577.53
91180.00	318.26	1630.31
101320.00	318.25	1663.33

Reference *https://www.doi.org/10.1016/j.jct.2012.09.027*

Sources

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Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol837.mol
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McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=837
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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

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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume