1-Butanol, 3-methyl-, propanoate

Other names:	1-Butanol, 3-methyl-, 1-propanoate
	3-METHYLBUTYL PROPANOATE
	3-Methyl-1-butyl propanoate
	3-Methylbutyl propionate
	ISOAMYL PROPANOATE
	ISOPENTYL PROPIONATE
	Isoamyl propionate
	Isopentyl alcohol, propionate
	Isopentyl propanoate
	NSC 7932
	Propionic acid, isopentyl ester
	iso-Amyl n-propionate
	propanoic acid, 3-methylbutyl ester
	propionic acid, isoamyl ester
Inchi:	InChI=1S/C8H16O2/c1-4-8(9)10-6-5-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	XAOGXQMKWQFZEM-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCC(=O)OCCC(C)C
Mol. weight [g/mol]:	144.21
CAS:	105-68-0

Physical Properties

Property code	Value	Unit	Source
gf	-219.88	kJ/mol	Joback Method
hf	-458.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	969.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	948.00		NIST Webbook

rinpol	960.00	NIST Webbook
rinpol	975.00	NIST Webbook
rinpol	971.00	NIST Webbook
rinpol	969.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	952.00	NIST Webbook
rinpol	972.00	NIST Webbook
rinpol	973.90	NIST Webbook
rinpol	974.00	NIST Webbook
rinpol	952.00	NIST Webbook
rinpol	952.00	NIST Webbook
rinpol	972.00	NIST Webbook
rinpol	949.00	NIST Webbook
rinpol	950.00	NIST Webbook
rinpol	969.00	NIST Webbook
rinpol	950.00	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	950.00	NIST Webbook
rinpol	947.00	NIST Webbook
rinpol	937.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	969.00	NIST Webbook
rinpol	955.00	NIST Webbook
rinpol	953.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	948.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	955.00	NIST Webbook
rinpol	948.00	NIST Webbook
rinpol	966.00	NIST Webbook
ripol	1198.00	NIST Webbook
ripol	1206.00	NIST Webbook
ripol	1176.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1188.00	NIST Webbook
ripol	1176.00	NIST Webbook
ripol	1181.00	NIST Webbook
ripol	1176.00	NIST Webbook
ripol	1192.00	NIST Webbook
ripol	1183.00	NIST Webbook

ripol	1184.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1186.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1200.00		NIST Webbook
tb	433.85 ± 0.25	K	NIST Webbook
tb	433.90	K	NIST Webbook
tb	433.87	K	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tb	431.65 ± 1.00	K	NIST Webbook
tb	433.50 ± 0.50	K	NIST Webbook
tb	433.40	K	KDB
tb	433.45 ± 1.00	K	NIST Webbook
tc	611.00	K	KDB
tc	611.39 ± 6.00	K	NIST Webbook
tf	237.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.23	J/mol×K	607.34	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	348.57	J/mol×K	637.16	Joback Method
cpl	285.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method

rhol	868.55	kg/m3	293.20	Liquid-liquid equilibrium data and thermophysical properties for ternary systems composed of water, acetic acid and different solvents
rhol	870.00	kg/m3	293.00	KDB
rhol	848.98	kg/m3	313.20	Liquid-liquid equilibrium data and thermophysical properties for ternary systems composed of water, acetic acid and different solvents

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	381.77	K	20.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	393.43	K	30.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa

tbp	402.13	K	40.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	409.26	K	50.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	415.18	K	60.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	420.42	K	70.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	425.06	K	80.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	

tbp	429.43	K	90.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	437.07	K	110.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	440.36	K	120.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	443.47	K	130.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	446.39	K	140.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	

tbp	449.17	K	150.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	451.76	K	160.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	454.42	K	170.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	456.84	K	180.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	
tbp	459.15	K	190.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa	

tbp	461.35	K	200.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50161e+01
Coeff. B	-3.87146e+03
Coeff. C	-6.15660e+01
Temperature range (K), min.	324.42
Temperature range (K), max.	460.49

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.55916e+01
Coeff. B	-5.65389e+03
Coeff. C	-1.33378e+00
Coeff. D	9.06163e-07
Temperature range (K), min.	281.15
Temperature range (K), max.	434.15

Sources

Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate andpropionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa:	https://www.doi.org/10.1016/j.fluid.2013.07.024
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1106.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105680&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-liquid equilibrium data and thermophysical properties for ternary systems composed of water, acetic acid and different solvents:	https://www.doi.org/10.1016/j.fluid.2018.10.021
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1106
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume