Butanoic acid, 3-methylbutyl ester

Other names:	3-Methyl-1-butyl butanoate
	3-Methylbutyl butanoate
	3-Methylbutyl butyrate
	3-Methylbutyl n-butyrate
	Butyric acid, isopentyl ester
	Isoamyl butanoate
	Isoamyl butylate
	Isoamyl butyrate
	Isoamyl-n-butyrate
	Isopentyl alcohol, butyrate
	Isopentyl butanoate
	Isopentyl butyrate
	Isopentyl-n-butyrate
	UN 2620
Inchi:	InChI=1S/C9H18O2/c1-4-5-9(10)11-7-6-8(2)3/h8H,4-7H2,1-3H3
InchiKey:	PQLMXFQTAMDXIZ-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	158.24
CAS:	106-27-4

Physical Properties

Property code	Value	Unit	Source
chl	-5491.10	kJ/mol	NIST Webbook
gf	-211.46	kJ/mol	Joback Method
hf	-479.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1054.00		NIST Webbook

rinpol	1039.00	NIST Webbook
rinpol	1039.40	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1062.00	NIST Webbook
rinpol	1056.00	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1055.50	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1056.00	NIST Webbook
rinpol	1056.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1054.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1013.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1039.40	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1039.00	NIST Webbook
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rinpol	1039.00	NIST Webbook
rinpol	1002.00	NIST Webbook
rinpol	1007.00	NIST Webbook
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rinpol	1002.00	NIST Webbook
rinpol	1041.00	NIST Webbook
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rinpol	1068.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1041.00	NIST Webbook
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ripol	1256.00	NIST Webbook
ripol	1266.00	NIST Webbook
ripol	1267.00	NIST Webbook
ripol	1270.00	NIST Webbook
ripol	1255.00	NIST Webbook
ripol	1255.00	NIST Webbook

ripol	1254.00		NIST Webbook
ripol	1262.00		NIST Webbook
tb	454.20 ± 0.25	K	NIST Webbook
tb	454.20 ± 0.30	K	NIST Webbook
tb	442.55 ± 1.00	K	NIST Webbook
tb	451.80 ± 0.50	K	NIST Webbook
tb	451.70 ± 0.50	K	NIST Webbook
tb	451.70 ± 0.50	K	NIST Webbook
tb	452.20	K	NIST Webbook
tc	618.83 ± 6.00	K	NIST Webbook
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method
dvisc	0.0006460	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006090	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005750	Pa×s	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006860	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0013170	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K	
dvisc	0.0011110	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K	
dvisc	0.0009520	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K	
dvisc	0.0008270	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K	

dvisc	0.0007310	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0007810	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0008360	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0008970	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0009670	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0005450	Pa×s	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0010440	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
hvapt	47.40	kJ/mol	373.00	NIST Webbook	
rhol	858.69	kg/m3	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K	

srf	0.02	N/m	338.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	348.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	288.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	358.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

srf	0.02	N/m	328.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51047e+01
Coeff. B	-4.02835e+03
Coeff. C	-6.68480e+01
Temperature range (K), min.	338.72
Temperature range (K), max.	478.19

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K:	https://www.doi.org/10.1021/je050170x
Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je050389b
NIST Webbook, Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106274&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Refractive Indices and Surface Tensions of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je0601208
Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters:	https://www.doi.org/10.1021/je050001c
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume