1-Butanol, 2-methyl-, acetate

Other names:	2-Methybutyl acetate
	2-Methyl-1-butanol acetate
	2-Methyl-1-butyl acetate
	2-Methylbutanol acetate
	2-Methylbutyl acetate
	2-methylbutyl ethanoate
	Acetic acid 2-methylbutyl ester
	Active amyl acetate
	acetic acid, 2-methylbutyl ester
	ethanoic acid, 2-methylbutyl ester
Inchi:	InChI=1S/C7H14O2/c1-4-6(2)5-9-7(3)8/h6H,4-5H2,1-3H3
InchiKey:	XHIUFYZDQBSEMF-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCC(C)COC(C)=O
Mol. weight [g/mol]:	130.18
CAS:	624-41-9

Physical Properties

Property code	Value	Unit	Source
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	883.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	879.00		NIST Webbook

rinpol	878.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	876.00	NIST Webbook
rinpol	877.00	NIST Webbook
rinpol	878.00	NIST Webbook
rinpol	872.00	NIST Webbook
rinpol	874.00	NIST Webbook
rinpol	852.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	884.50	NIST Webbook
rinpol	880.00	NIST Webbook
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rinpol	882.00	NIST Webbook
rinpol	876.00	NIST Webbook
rinpol	878.00	NIST Webbook
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rinpol	880.00	NIST Webbook
rinpol	874.00	NIST Webbook
rinpol	877.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	861.00	NIST Webbook
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rinpol	886.00	NIST Webbook

rinpol	886.00	NIST Webbook
ripol	1126.00	NIST Webbook
ripol	1132.00	NIST Webbook
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ripol	1134.00	NIST Webbook
ripol	1128.00	NIST Webbook
ripol	1125.00	NIST Webbook
ripol	1125.00	NIST Webbook
ripol	1116.00	NIST Webbook
ripol	1111.00	NIST Webbook
ripol	1115.00	NIST Webbook
ripol	1119.00	NIST Webbook
ripol	1127.00	NIST Webbook
ripol	1126.00	NIST Webbook
ripol	1112.00	NIST Webbook
ripol	1112.00	NIST Webbook
ripol	1116.00	NIST Webbook
ripol	1119.00	NIST Webbook
ripol	1128.00	NIST Webbook
ripol	1081.00	NIST Webbook
ripol	1121.00	NIST Webbook
ripol	1119.00	NIST Webbook
ripol	1128.00	NIST Webbook
ripol	1126.00	NIST Webbook
ripol	1165.00	NIST Webbook
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ripol	1131.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1131.00	NIST Webbook
ripol	1114.00	NIST Webbook
ripol	1131.00	NIST Webbook
ripol	1134.00	NIST Webbook
ripol	1134.00	NIST Webbook
ripol	1096.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1125.00	NIST Webbook

tb	413.15 ± 1.00	K	NIST Webbook
tb	411.38	K	Isobaric Vapor Liquid Equilibria for the Binary and Ternary Systems of 2-Methyl-1-butanol, 2-Methyl-butanol Acetate, and Dimethylformamide (DMF) at 101.3 kPa
tb	414.00	K	NIST Webbook
tb	412.00 ± 2.00	K	NIST Webbook
tc	615.76	K	Joback Method
tf	225.81	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/mol×K	435.41	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	301.45	J/mol×K	615.76	Joback Method
dvisc	0.0047724	Pa×s	225.81	Joback Method
dvisc	0.0021099	Pa×s	260.74	Joback Method
dvisc	0.0011312	Pa×s	295.68	Joback Method
dvisc	0.0006919	Pa×s	330.61	Joback Method
dvisc	0.0004649	Pa×s	365.54	Joback Method
dvisc	0.0003348	Pa×s	400.48	Joback Method
dvisc	0.0002542	Pa×s	435.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51408e+01
Coeff. B	-3.76699e+03
Coeff. C	-5.60060e+01

Temperature range (K), min.	309.62
Temperature range (K), max.	439.25

Sources

Isobaric Vapor Liquid Equilibria for the Binary and Ternary Systems of 2-Methyl-1-butanol, 2-Methyl-butanol Acetate, and Dimethylformamide (DMF) at 101.3 kPa.	https://www.doi.org/10.1021/je3012925
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624419&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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