

2-Butanol, 2-methyl-, acetate

Other names:	1,1-Dimethylpropyl acetate 1,1-dimethylpropyl ethanoate 2-methyl-2-butyl acetate Acetic acid, 1,1-dimethylpropyl ester CH ₃ C(O)OC(CH ₃) ₂ CH ₂ CH ₃ ethanoic acid, 1,1-dimethylpropyl ester tert-Amyl acetate tert-Amyl ethanoate tert-Pentyl Acetate tert-Pentyl Alcohol, acetate
Inchi:	InChI=1S/C7H14O2/c1-5-7(3,4)9-6(2)8/h5H2,1-4H3
InchiKey:	JCCIFDCPHCKATH-UHFFFAOYSA-N
Formula:	C ₇ H ₁₄ O ₂
SMILES:	CCC(C)(C)OC(C)=O
Mol. weight [g/mol]:	130.18
CAS:	625-16-1

Physical Properties

Property code	Value	Unit	Source
chl	-4173.60 ± 1.50	kJ/mol	NIST Webbook
gf	-223.02	kJ/mol	Joback Method
hf	-539.00 ± 1.50	kJ/mol	NIST Webbook
hfl	-581.80 ± 1.50	kJ/mol	NIST Webbook
hfus	9.26	kJ/mol	Joback Method
hvap	40.30	kJ/mol	NIST Webbook
hvap	42.80 ± 0.34	kJ/mol	NIST Webbook
hvap	42.80	kJ/mol	NIST Webbook
hvap	42.80 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.738		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	753.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	793.00		NIST Webbook
ripol	1003.00		NIST Webbook

ripol	1003.00		NIST Webbook
ripol	917.00		NIST Webbook
tb	396.65 ± 0.60	K	NIST Webbook
tb	397.65 ± 1.00	K	NIST Webbook
tb	393.15 ± 1.00	K	NIST Webbook
tc	620.42	K	Joback Method
tf	243.23	K	Joback Method
vc	0.441	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.05	J/mol×K	432.62	Joback Method
cpg	253.38	J/mol×K	463.92	Joback Method
cpg	265.15	J/mol×K	495.22	Joback Method
cpg	276.37	J/mol×K	526.52	Joback Method
cpg	287.06	J/mol×K	557.82	Joback Method
cpg	297.22	J/mol×K	589.12	Joback Method
cpg	306.89	J/mol×K	620.42	Joback Method
dvisc	0.0047587	Paxs	243.23	Joback Method
dvisc	0.0022582	Paxs	274.80	Joback Method
dvisc	0.0012495	Paxs	306.36	Joback Method
dvisc	0.0007722	Paxs	337.93	Joback Method
dvisc	0.0005181	Paxs	369.49	Joback Method
dvisc	0.0003702	Paxs	401.06	Joback Method
dvisc	0.0002778	Paxs	432.62	Joback Method
hvapt	42.80	kJ/mol	209.00	NIST Webbook
pvap	0.51	kPa	277.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.40	kPa	274.00	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.44	kPa	275.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.39	kPa	273.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.52	kPa	278.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.57	kPa	279.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.64	kPa	281.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.72	kPa	283.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.74	kPa	283.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.88	kPa	286.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.95	kPa	288.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	1.05	kPa	289.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.22	kPa	292.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.34	kPa	293.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.49	kPa	295.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.70	kPa	298.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.79	kPa	298.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.08	kPa	301.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.33	kPa	303.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	2.42	kPa	304.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.83	kPa	307.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.99	kPa	308.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52581e+01
Coeff. B	-3.67169e+03
Coeff. C	-5.15580e+01
Temperature range (K), min.	296.82
Temperature range (K), max.	420.70

Sources

Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters:

<https://www.doi.org/10.1016/j.fluid.2008.02.001>

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=C625161&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/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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
hfl:	Liquid phase 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
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

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