Allyl alcohol

Other names:	1-Hydroxy-2-propene
	1-Propenol-3
	1-Propenol-3-ol
	1-propen-3-ol
	2-Propene-1-ol
	2-Propenyl alcohol
	2-propen-1-ol
	2-propen-1-ol (allyl alcohol)
	2-propenol
	3-Hydroxy-1-propene
	3-hydroxypropene
	AA
	Alcool allilco
	Alcool allylique
	Allilowy alkohol
	Allyl al
	Allylalkohol
	Allylic alcohol
	CH2=CHCH2OH
	NSC 6526
	PROPENYLALCOHOL
	Propen-1-ol-3
	Propenol-3
	Propenyl alcohol
	Rcra waste number P005
	Shell Unkrauttod A
	Shell unkrautted A
	UN 1098
	Vinylcarbinol
	Weed drench
	prop-2-en-1-ol
Inchi:	InChI=1S/C3H6O/c1-2-3-4/h2,4H,1,3H2
InchiKey:	XXROGKLTLUQVRX-UHFFFAOYSA-N
Formula:	C3H6O
SMILES:	C=CCO
Mol. weight [g/mol]:	58.08
CAS:	107-18-6

Physical Properties

Property code	Value	Unit	Source
af	0.5540		KDB
aigt	715.93	K	KDB
fll	2.50	% in Air	KDB
flu	18.00	% in Air	KDB
fpc	305.37	K	KDB
fpo	295.37	K	KDB
gf	-71.30	kJ/mol	KDB
hf	-132.10	kJ/mol	KDB
hf	-123.60 ± 1.50	kJ/mol	NIST Webbook
hfus	6.33	kJ/mol	Joback Method
hvap	44.80	kJ/mol	NIST Webbook
hvap	47.00 ± 1.00	kJ/mol	NIST Webbook
hvap	47.30	kJ/mol	NIST Webbook
hvap	46.10	kJ/mol	NIST Webbook
ie	9.63	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.67 ± 0.03	eV	NIST Webbook
ie	10.22	eV	NIST Webbook
ie	9.67 ± 0.05	eV	NIST Webbook
log10ws	0.73		Cheméo Relay (1.0)
logp	0.165		Crippen Method
mcvol	54.700	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=1)		KDB
pc	5310.00	kPa	KDB
pc	5640.00	kPa	Critical Point and Vapor Pressure Measurements for Seven Compounds by a Low Residence Time Flow Method
rinpol	534.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	540.00		NIST Webbook

rinpol	555.00	NIST Webbook
rinpol	558.00	NIST Webbook
rinpol	555.00	NIST Webbook
rinpol	555.00	NIST Webbook
rinpol	555.00	NIST Webbook
rinpol	537.00	NIST Webbook
rinpol	556.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	545.00	NIST Webbook
rinpol	543.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	519.00	NIST Webbook
rinpol	501.00	NIST Webbook
rinpol	539.00	NIST Webbook
rinpol	512.00	NIST Webbook
rinpol	526.00	NIST Webbook
rinpol	549.00	NIST Webbook
rinpol	532.00	NIST Webbook
rinpol	546.00	NIST Webbook
rinpol	498.00	NIST Webbook
ripol	1128.00	NIST Webbook
ripol	1125.00	NIST Webbook
ripol	1136.00	NIST Webbook
ripol	1116.00	NIST Webbook
ripol	1116.00	NIST Webbook
ripol	1109.00	NIST Webbook
ripol	1109.00	NIST Webbook
ripol	1107.00	NIST Webbook
ripol	1125.00	NIST Webbook
ripol	1130.00	NIST Webbook
ripol	1125.00	NIST Webbook
ripol	1100.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1119.00	NIST Webbook
ripol	1124.00	NIST Webbook
ripol	1124.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1144.00	NIST Webbook
ripol	1111.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1108.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1122.00	NIST Webbook
ripol	1100.00	NIST Webbook

ripol	1138.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1098.00		NIST Webbook
ripol	1128.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1130.00		NIST Webbook
tb	369.90	K	Measurement and Correlation of Isobaric Vapor-Liquid Equilibrium for Binary Systems of Allyl Alcohol with Isobutyl Acetate, Butyl Acetate, and Butyl Propionate at 101.3 kPa
tb	369.75	K	Vapor-Liquid Equilibrium for Binary Systems of Allyl Alcohol + Water and Allyl Alcohol + Benzene at 101.3 kPa
tb	369.60 ± 2.00	K	NIST Webbook
tb	370.10 ± 0.50	K	NIST Webbook
tb	370.10 ± 0.30	K	NIST Webbook
tb	369.95	K	Separation of azeotrope (allyl alcohol + water): Isobaric vapour-liquid phase equilibrium measurements and extractive distillation
tb	370.00	K	NIST Webbook
tb	370.30	K	NIST Webbook
tb	369.94	K	Isobaric Vapor-Liquid Phase Equilibrium Measurements for Allyl Alcohol with Chloroform, Ethyl Acetate, and Methyl Propionate at 101.3 kPa
tb	370.25 ± 0.30	K	NIST Webbook
tb	370.00 ± 0.40	K	NIST Webbook
tb	370.23	K	KDB
tb	370.00 ± 0.50	K	NIST Webbook
tb	369.62 ± 0.50	K	NIST Webbook
tb	370.23 ± 0.30	K	NIST Webbook
tb	370.07 ± 0.20	K	NIST Webbook
tc	545.10	K	NIST Webbook
tc	545.10	K	NIST Webbook
tc	545.00	K	KDB
tf	144.00	K	KDB
vc	0.203	m3/kmol	KDB
zc	0.2384660		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.33	J/mol×K	356.90	Joback Method
cpg	115.41	J/mol×K	522.27	Joback Method
cpg	111.36	J/mol×K	494.71	Joback Method
cpg	107.13	J/mol×K	467.15	Joback Method
cpg	102.72	J/mol×K	439.59	Joback Method
cpg	98.12	J/mol×K	412.02	Joback Method
cpg	93.33	J/mol×K	384.46	Joback Method
cpl	141.93	J/mol×K	288.72	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	149.16	J/mol×K	304.04	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	138.90	J/mol×K	298.00	NIST Webbook
cpl	160.30	J/mol×K	324.46	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	160.14	J/mol×K	324.46	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	134.94	J/mol×K	273.41	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	134.61	J/mol×K	273.41	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	137.19	J/mol×K	278.52	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	137.35	J/mol×K	278.52	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	139.43	J/mol×K	283.62	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols

cpl	139.18	J/mol×K	283.62	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	157.06	J/mol×K	319.35	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	141.68	J/mol×K	288.72	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	144.34	J/mol×K	293.83	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	144.17	J/mol×K	293.83	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	146.67	J/mol×K	298.93	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	146.50	J/mol×K	298.93	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	157.23	J/mol×K	319.35	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	149.08	J/mol×K	304.04	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	152.32	J/mol×K	309.14	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	151.82	J/mol×K	309.14	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	154.82	J/mol×K	314.25	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
cpl	154.40	J/mol×K	314.25	Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols
dvisc	0.0003781	Pa×s	356.90	Joback Method
dvisc	0.0006605	Pa×s	327.86	Joback Method
dvisc	0.0028903	Pa×s	269.76	Joback Method
dvisc	0.0078973	Pa×s	240.72	Joback Method
dvisc	0.0284333	Pa×s	211.67	Joback Method

dvisc	0.1538622	Pa×s	182.63	Joback Method
dvisc	0.0012861	Pa×s	298.81	Joback Method
hvapt	46.70	kJ/mol	311.50	NIST Webbook
hvapt	39.96	kJ/mol	369.70	KDB
hvapt	44.60	kJ/mol	325.00	NIST Webbook
pvap	15.67	kPa	326.70	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol
pvap	52.33	kPa	353.15	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol
pvap	518.11	kPa	423.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
pvap	109.95	kPa	373.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
pvap	518.64	kPa	423.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
pvap	109.94	kPa	373.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
pvap	520.67	kPa	423.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation

pvap	113.10	kPa	373.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
pvap	58.11	kPa	355.70	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol
pvap	53.30	kPa	353.59	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol
pvap	101.30	kPa	369.75	Vapor-Liquid Equilibrium for Binary Systems of Allyl Alcohol + Water and Allyl Alcohol + Benzene at 101.3 kPa
pvap	101.30	kPa	369.94	Isobaric Vapor-Liquid Phase Equilibrium Measurements for Allyl Alcohol with Chloroform, Ethyl Acetate, and Methyl Propionate at 101.3 kPa
pvap	6.95	kPa	311.42	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol
pvap	7.67	kPa	313.15	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol
pvap	8.87	kPa	315.81	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol
pvap	11.08	kPa	319.97	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol

pvap	52.34	kPa	353.15	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
pvap	20.19	kPa	331.84	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
pvap	21.51	kPa	333.15	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
pvap	22.60	kPa	334.20	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
pvap	26.94	kPa	337.96	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
pvap	31.72	kPa	341.54	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
pvap	35.82	kPa	344.27	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
pvap	40.30	kPa	346.97	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
pvap	48.61	kPa	351.37	Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol	
rfi	1.41280		293.15	Solubility of hydrogen in bio-oil compounds	
rhol	855.00	kg/m3	288.00	KDB	

rhol	854.00	kg/m3	293.15	Isobaric Vapor Liquid Equilibrium for Binary Systems of Allyl Alcohol with Water, Methanol, and Ethanol at 101.3 kPa
rhol	832.63	kg/m3	318.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure
rhol	837.13	kg/m3	313.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure
rhol	841.59	kg/m3	308.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure
rhol	846.02	kg/m3	303.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure

rhol	850.40	kg/m3	298.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure
rhol	855.00	kg/m3	293.15	Salts effect on isobaric vapor-liquid equilibrium for separation of the azeotropic mixture allyl alcohol + water
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59415e+01
Coeff. B	-3.58605e+03
Coeff. C	-5.33010e+01
Temperature range (K), min.	282.38
Temperature range (K), max.	545.10

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.40943e+01
Coeff. B	-6.87755e+03
Coeff. C	-5.24079e+00
Coeff. D	6.03381e-07
Temperature range (K), min.	144.15
Temperature range (K), max.	545.05

Sources

Salts effect on isobaric vapor-liquid equilibrium for separation of the azeotropic mixture allyl alcohol + water:	https://www.doi.org/10.1016/j.fluid.2017.10.025
Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and water:	https://www.doi.org/10.1016/j.tca.2015.04.027
Solubility of hydrogen in bio-oil compounds:	https://www.doi.org/10.1016/j.jct.2016.07.010
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cetyl 3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure:	https://www.doi.org/10.1021/acs.jced.8b00908
Isobaric Vapor-Liquid Phase Equilibrium Measurements for Allyl Alcohol + Chloroform, Ethyl Acetate, and 1-Propanol:	https://www.doi.org/10.1021/je0499519
Vapor-Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol at 101.3 kPa:	https://www.doi.org/10.1021/je0502647
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 2-Chloropropane in 2-Propanol:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=895
KDB Vapor Pressure Data:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.doi.org/10.1021/acs.jced.5b01048
Isobaric Vapor-Liquid Equilibrium for Binary Systems of Allyl Alcohol with Water, Methanol, and Ethanol at 101.3 kPa:	https://www.doi.org/10.1021/je060088h
Measurements for Seven Compounds by a Low-Residence-Time Flow Method:	https://www.doi.org/10.1016/j.tca.2014.03.043
Heat Capacities of 2-Propenol and Selected Cyclohexylalcohols:	https://www.cheric.org/files/research/kdb/mol/mol895.mol
KDB:	
Cheméo Relay (1.0):	
Separation of azeotrope (allyl alcohol + water): Isobaric vapour-liquid phase equilibrium measurements and extractive distillation:	https://www.doi.org/10.1016/j.jct.2017.11.009
Cheméo Relay (1.0, beta):	
Vapor-Liquid Equilibrium for Binary Systems of Allyl Alcohol + Water and Allyl Alcohol + Benzene at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.6b00893
4-Chloroacetophenone to 2-Propenyl-1-ol:	https://en.wikipedia.org/wiki/Joback_method
Joback Method:	https://www.doi.org/10.1021/je400885z
Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107186&Units=SI
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	https://www.doi.org/10.1021/acs.jced.7b01024
Measurement and Correlation of Isobaric Vapor-Liquid Equilibrium for Binary Systems of Allyl Alcohol with Isobutyl Acetate, Butyl Acetate, and Butyl Propionate at 101.3 kPa:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The Yaws Handbook of Vapor Pressure:	

Legend

af:	Acentric Factor
aigt:	Autoignition Temperature
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
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
ie:	Ionization energy
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
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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
zc:	Critical Compressibility