Acetic acid ethenyl ester

Other names:	1-ACETOXYETHYLENE
	Acetate de vinyle
	Acetic acid vinyl ester
	Acetic acid, ethylene ether
	Acetoxyethene
	CH3CO2CH=CH2
	ETHENYL ETHANOATE
	Ethanoic acid, ethenyl ester
	Ethenyl acetate
	Everflex 81L
	NSC 8404
	Octan winylu
	Plyamul 40305-00
	Unocal 76 Res 6206
	Unocal 76 Res S-55
	VAC
	VINYL ETHANOATE
	Vinile (acetato di)
	Vinnapas A 50
	Vinyl A monomer
	Vinyl acetate
	Vinyl acetate h.q.
	Vinyl acetate monomer
	Vinyl ester of acetic acid
	Vinylacetaat
	Vinylacetat
	Vinyle (acetate de)
	Vinylester kyseliny octove
	VyAc
	Zeset T
	acetic acid, vinyl ester
Inchi:	InChI=1S/C4H6O2/c1-3-6-4(2)5/h3H,1H2,2H3
InchiKey:	XTXRWKRVRITETP-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	C=COC(C)=O
Mol. weight [g/mol]:	86.09
CAS:	108-05-4

Physical Properties

Property code	Value	Unit	Source
af	0.3400		KDB
affp	813.90	kJ/mol	NIST Webbook
aigt	699.82	K	KDB
basg	782.90	kJ/mol	NIST Webbook
chl	-2086.00 ± 10.00	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
fll	2.60	% in Air	KDB
flu	13.40	% in Air	KDB
fpc	268.15	K	KDB
fpo	265.37	K	KDB
gf	-163.28	kJ/mol	Joback Method
gyrad	3.0890		KDB
hf	-316.00	kJ/mol	KDB
hf	-313.60	kJ/mol	NIST Webbook
hf	-309.00 ± 10.00	kJ/mol	NIST Webbook
hfl	-346.00 ± 10.00	kJ/mol	NIST Webbook
hfl	-350.80	kJ/mol	NIST Webbook
hfus	7.62	kJ/mol	Joback Method
hvap	37.20 ± 0.84	kJ/mol	NIST Webbook
ie	9.85	eV	NIST Webbook
ie	9.19 ± 0.05	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.85 ± 0.05	eV	NIST Webbook
log10ws	-0.71		Crippen Method
logp	0.693		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	4185.00 ± 9.00	kPa	NIST Webbook
pc	4350.00	kPa	KDB
rinpol	560.00		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	527.00		NIST Webbook

rinpol	529.00		NIST Webbook
rinpol	545.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	570.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	570.00		NIST Webbook
ripol	878.00		NIST Webbook
tb	345.95	K	Isobaric Vapor Liquid Equilibrium of Binary Mixtures of Vinyl Acetate and Ethyl Formate with Cumene at 97.3 kPa
tb	345.75	K	Vapor Liquid Equilibrium at p/kPa = 101.3 of the Binary Mixtures of Ethenyl Acetate with Methanol and Butan-1-ol
tb	346.10	K	Vapor-Liquid Equilibrium and Mixing Properties of Methanol + Diethyl Carbonate and Vinyl Acetate + Diethyl Carbonate Systems
tb	346.00	K	KDB
tc	519.13 ± 0.40	K	NIST Webbook
tc	525.00	K	KDB
tf	172.95 ± 0.30	K	NIST Webbook
tf	173.00	K	KDB
tf	180.35	K	NIST Webbook
vc	0.265	m3/kmol	KDB
zc	0.2640820		KDB
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.32	J/mol×K	363.89	Joback Method
cpg	122.50	J/mol×K	394.42	Joback Method
cpg	128.49	J/mol×K	424.95	Joback Method
cpg	134.29	J/mol×K	455.47	Joback Method
cpg	139.91	J/mol×K	486.00	Joback Method
cpg	145.34	J/mol×K	516.53	Joback Method

cpg	150.58	J/mol×K	547.06	Joback Method
cpl	169.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0021165	Pa×s	205.24	Joback Method
dvisc	0.0012203	Pa×s	231.68	Joback Method
dvisc	0.0007877	Pa×s	258.12	Joback Method
dvisc	0.0005515	Pa×s	284.56	Joback Method
dvisc	0.0004102	Pa×s	311.01	Joback Method
dvisc	0.0003197	Pa×s	337.45	Joback Method
dvisc	0.0002583	Pa×s	363.89	Joback Method
hfust	8.46	kJ/mol	180.60	NIST Webbook
hfust	8.46	kJ/mol	180.60	NIST Webbook
hvapt	34.40	kJ/mol	320.00	NIST Webbook
hvapt	31.40	kJ/mol	347.50	NIST Webbook
pvap	101.30	kPa	346.10	Vapor-Liquid Equilibrium and Mixing Properties of Methanol + Diethyl Carbonate and Vinyl Acetate + Diethyl Carbonate Systems
pvap	97.30	kPa	344.68	Vapor-Liquid Equilibria and Excess Properties of the Binary System Vinyl Acetate + p-Xylene
pvap	101.30	kPa	345.75	Vapor Liquid Equilibrium at p/kPa = 101.3 of the Binary Mixtures of Ethenyl Acetate with Methanol and Butan-1-ol
rfi	1.39253		298.15	Density, Refractive Index, Speed of Sound, and Vapor-Liquid Equilibria for Binary Mixtures of Methanol + Vinyl Propionate and Vinyl Acetate + Vinyl Propionate. Vapor Pressures of Vinyl Propionate

rfi	1.39260		293.15	Measurement and Modeling of Liquid Liquid Equilibrium for the Systems Vinyl Acetate + Acetic Acid/Ethanol + Water at 298.15 and 308.15 K	
rhol	913.50	kg/m3	308.15	Density, viscosity, and speed of sound of binary liquid mixtures of vinyl acetate with butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether	
rhol	925.77	kg/m3	298.15	Densities and derived thermodynamic properties of the binary systems of 1,1-dimethylethyl methyl ether with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at T = (298.15 and 308.15) K	
rhol	932.00	kg/m3	293.00	KDB	
rhol	913.13	kg/m3	308.15	Densities and derived thermodynamic properties of the binary systems of 1,1-dimethylethyl methyl ether with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at T = (298.15 and 308.15) K	

rhol	931.95	kg/m3	293.15	Density, excess volume, and excess coefficient of thermal expansion of the binary systems of dimethyl carbonate with butyl methacrylate, allyl methacrylate, styrene, and vinyl acetate at T = (293.15, 303.15, and 313.15) K
rhol	919.09	kg/m3	303.15	Density, excess volume, and excess coefficient of thermal expansion of the binary systems of dimethyl carbonate with butyl methacrylate, allyl methacrylate, styrene, and vinyl acetate at T = (293.15, 303.15, and 313.15) K
rhol	906.12	kg/m3	313.15	Density, excess volume, and excess coefficient of thermal expansion of the binary systems of dimethyl carbonate with butyl methacrylate, allyl methacrylate, styrene, and vinyl acetate at T = (293.15, 303.15, and 313.15) K
rhol	919.40	kg/m3	303.15	Density, viscosity, and speed of sound of binary liquid mixtures of vinyl acetate with butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether

rhol	913.13	kg/m3	308.15	Densities, isobaric thermal compressibilities and derived thermodynamic properties of the binary systems of cyclohexane with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at t = (298.15 and 308.15)K
rhol	925.77	kg/m3	298.15	Densities, isobaric thermal compressibilities and derived thermodynamic properties of the binary systems of cyclohexane with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at t = (298.15 and 308.15)K
rhol	907.30	kg/m3	313.15	Density, viscosity, and speed of sound of binary liquid mixtures of vinyl acetate with butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48909e+01
Coeff. B	-3.20824e+03
Coeff. C	-3.33880e+01
Temperature range (K), min.	253.08
Temperature range (K), max.	519.13

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.86249e+01
Coeff. B	-5.47773e+03
Coeff. C	-4.86787e+00
Coeff. D	2.36709e-06
Temperature range (K), min.	180.35
Temperature range (K), max.	524.00

Sources

Vapor-Liquid Equilibrium and Mixing Properties of Methanol + Diethyl Carbonate and Vinyl Acetate + Diethyl Carbonate Systems:	https://www.doi.org/10.1021/je049544x
Solubility of Flavonoids in Organic Solvents:	https://www.doi.org/10.1021/je7001094
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Isobaric Vapor Liquid Equilibrium of Binary Mixtures of Vinyl Acetate and Ethyl Formate with Cumene at 97.3 kPa:	https://www.doi.org/10.1021/je7004402
Densities, isobaric thermal compressibilities and derived thermodynamic properties of the binary systems of cyclohexane with allyl methacrylate, butyl methacrylate, methyl methacrylate and vinyl acetate at t = (298.15 and 308.15) K:	https://www.doi.org/10.1016/j.tca.2005.06.007
Thermodynamics and activity coefficients at infinite dilution for organic solutes, water and diols in the ionic liquid [illegible] bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2014.04.024
Vapor-Liquid Equilibria and Excess Properties of the Binary System Vinyl [illegible]:	https://www.doi.org/10.1021/je050162g
New ionic liquid [illegible] in bio-butanol extraction on investigation of limiting activity coefficients:	https://www.doi.org/10.1016/j.fluid.2018.07.028
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1167
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The study of excess molar volumes and related properties for binary mixtures containing benzyl alcohol and 1,3-dichloro-2-propanol with vinyl acetate, ethyl acetate and t-butyl acetate at T = 293.15 to 313.15 K and P = 0.087 MPa:	https://www.doi.org/10.1016/j.tca.2016.04.001
Separation of binary mixtures based on limiting activity coefficients data using specific ammonium-based ionic liquid and modelling of thermodynamic functions:	https://www.doi.org/10.1016/j.fluid.2017.12.029
Measurement and Modeling of Liquid-Liquid Equilibrium for the Systems Vinyl Acetate + Acetic Acid/Ethanol + Water at 298.15 and 308.15 K:	https://www.doi.org/10.1021/acs.jced.6b00794
Density, Refractive Index, Speed of Sound, and Vapor-Liquid Equilibria for Binary Mixtures of Methanol + Vinyl Propionate and Vinyl Acetate + Vinyl Propionate. Vapor Pressures of Vinyl Propionate:	https://www.doi.org/10.1021/je049909d
Vapor-Liquid Equilibrium at p/kPa = 101.3 of the Binary Mixtures of Ethenyl Acetate with Methanol and Butan-1-ol:	https://www.doi.org/10.1021/je300835h
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-3-methylimidazolium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2013.05.008
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108054&Units=SI
Bubble-Point Measurement for CO2 + Vinyl Acetate and CO2 + Vinyl Acrylate Systems at High Pressures.:	https://www.doi.org/10.1021/je0201121
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Density, viscosity, and speed of sound of binary liquid mixtures of vinyl acetate with butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether:	https://www.doi.org/10.1016/j.jct.2019.04.018
Ammonium ionic liquids in extraction of bio-butan-1-ol from water phase using activity coefficients at infinite dilution:	https://www.doi.org/10.1016/j.fluid.2018.09.024
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1167.mol
The use of ionic liquids for separation of binary hydrocarbons mixtures based on gamma infinity data measurements:	https://www.doi.org/10.1016/j.jct.2018.07.024
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 4-(3-hydroxypropyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)amide:	https://www.doi.org/10.1016/j.jct.2015.02.024
Separation of binary mixtures hexane/hex-1-ene, cyclohexane/cyclohexene and ethylbenzene/styrene based on gamma infinity data measurements:	https://www.doi.org/10.1016/j.jct.2017.11.017
Activity coefficients at infinite dilution, physicochemical and thermodynamic properties for organic solutes and water in the ionic liquid ethyl-dimethyl-(2-methoxyethyl)ammonium trifluorotris-(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2015.05.022

Thermodynamic study of molecular interaction-selectivity in separation processes based on limiting activity coefficients: https://www.doi.org/10.1016/j.jct.2018.02.014

Density, excess volume and excess coefficient of thermal expansion of the binary systems of dimethyl carbonate with butyl methacrylate, allyl methacrylate, ethyl acrylate and vinyl acetate at T = (298.15 and 308.15) K: https://www.doi.org/10.1016/j.jct.2008.06.017

Phase equilibria of the ternary system vinyl acetate + ethyl acrylate + allyl methacrylate at 313.15 K: https://www.doi.org/10.1016/j.fluid.2008.02.010

Densities and derived thermodynamic properties of the binary systems of 1,1-dimethylethyl methyl ether with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at T = (298.15 and 308.15) K: https://www.doi.org/10.1016/j.jct.2004.11.012

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter

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https://www.chemeo.com/cid/38-615-7/Acetic-acid-ethenyl-ester.pdf
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