Acetaldehyde

Other names:	ACETIC ALDEHYDE
	Acetaldehyd
	Acetylaldehyde
	Aldehyde acetique
	Aldeide acetica
	CH3CHO
	ETHANAL
	Ethyl aldehyde
	NCI-C56326
	NSC 7594
	Octowy aldehyd
	Rcra waste number U001
	UN 1089
	methanecarbaldehyde
Inchi:	InChI=1S/C2H4O/c1-2-3/h2H,1H3
InchiKey:	IKHGUXGNUITLKF-UHFFFAOYSA-N
Formula:	C2H4O
SMILES:	CC=O
Mol. weight [g/mol]:	44.05
CAS:	75-07-0

Physical Properties

Property code	Value	Unit	Source
af	0.3030		KDB
affp	768.50	kJ/mol	NIST Webbook
aigt	458.15	K	KDB
basg	736.50	kJ/mol	NIST Webbook
dm	2.50	debye	KDB
ea	3.50e-04	eV	NIST Webbook
fll	4.00	% in Air	KDB
flu	60.00	% in Air	KDB
fpc	223.15	K	KDB
fpo	235.37	K	KDB
gf	-133.40	kJ/mol	KDB
gyrad	2.0210		KDB
hf	-170.70 ± 1.50	kJ/mol	NIST Webbook
hf	-164.40	kJ/mol	KDB

hfl	-196.40 ± 1.50	kJ/mol	NIST Webbook
hfus	3.23	kJ/mol	Joback Method
hvap	26.12	kJ/mol	NIST Webbook
hvap	25.70	kJ/mol	NIST Webbook
hvap	26.90	kJ/mol	NIST Webbook
ie	10.25 ± 0.03	eV	NIST Webbook
ie	10.21 ± 0.01	eV	NIST Webbook
ie	10.20 ± 0.03	eV	NIST Webbook
ie	10.23 ± 0.00	eV	NIST Webbook
ie	10.23 ± 0.00	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.20 ± 0.03	eV	NIST Webbook
ie	10.22 ± 0.01	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.22	eV	NIST Webbook
ie	10.23	eV	NIST Webbook
ie	10.20 ± 0.02	eV	NIST Webbook
ie	10.90	eV	NIST Webbook
ie	10.22	eV	NIST Webbook
ie	10.26	eV	NIST Webbook
ie	10.14 ± 0.02	eV	NIST Webbook
ie	10.22	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.23 ± 0.01	eV	NIST Webbook
ie	10.23	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.20 ± 0.02	eV	NIST Webbook
ie	10.21	eV	NIST Webbook
ie	10.19	eV	NIST Webbook
ie	10.22 ± 0.01	eV	NIST Webbook
ie	10.23 ± 0.00	eV	NIST Webbook
ie	10.24 ± 0.02	eV	NIST Webbook
ie	10.22 ± 0.01	eV	NIST Webbook
ie	10.22 ± 0.01	eV	NIST Webbook
ie	10.24	eV	NIST Webbook
log10ws	0.06		Crippen Method
logp	0.205		Crippen Method
mcvol	40.610	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	5570.00	kPa	KDB
rhoc	285.90 ± 4.41	kg/m3	NIST Webbook

rinpol	380.00	NIST Webbook
rinpol	381.00	NIST Webbook
rinpol	381.00	NIST Webbook
rinpol	363.00	NIST Webbook
rinpol	418.00	NIST Webbook
rinpol	360.00	NIST Webbook
rinpol	356.00	NIST Webbook
rinpol	365.00	NIST Webbook
rinpol	372.00	NIST Webbook
rinpol	412.00	NIST Webbook
rinpol	412.00	NIST Webbook
rinpol	360.00	NIST Webbook
rinpol	400.00	NIST Webbook
rinpol	363.00	NIST Webbook
rinpol	381.00	NIST Webbook
rinpol	427.00	NIST Webbook
rinpol	372.00	NIST Webbook
rinpol	360.00	NIST Webbook
rinpol	373.00	NIST Webbook
rinpol	352.00	NIST Webbook
rinpol	342.00	NIST Webbook
rinpol	352.00	NIST Webbook
rinpol	372.00	NIST Webbook
rinpol	404.00	NIST Webbook
rinpol	400.00	NIST Webbook
rinpol	363.00	NIST Webbook
rinpol	363.00	NIST Webbook
rinpol	410.00	NIST Webbook
rinpol	363.00	NIST Webbook
rinpol	372.00	NIST Webbook
rinpol	381.00	NIST Webbook
rinpol	352.00	NIST Webbook
rinpol	400.00	NIST Webbook
rinpol	372.00	NIST Webbook
rinpol	418.00	NIST Webbook
rinpol	360.88	NIST Webbook
rinpol	360.50	NIST Webbook
rinpol	361.00	NIST Webbook
rinpol	346.00	NIST Webbook
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rinpol	360.37	NIST Webbook
rinpol	360.64	NIST Webbook
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ripol	700.00	NIST Webbook
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ripol	716.60	NIST Webbook
ripol	748.00	NIST Webbook
ripol	702.00	NIST Webbook
ripol	727.00	NIST Webbook
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ripol	710.00	NIST Webbook
ripol	718.80	NIST Webbook
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ripol	655.00	NIST Webbook
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ripol	714.00	NIST Webbook
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ripol	724.00	NIST Webbook
ripol	677.00	NIST Webbook
ripol	694.00	NIST Webbook
ripol	669.00	NIST Webbook
ripol	677.00	NIST Webbook
ripol	655.00	NIST Webbook
ripol	668.00	NIST Webbook
ripol	669.00	NIST Webbook
ripol	724.00	NIST Webbook
ripol	709.00	NIST Webbook
ripol	710.00	NIST Webbook
ripol	716.00	NIST Webbook
ripol	716.00	NIST Webbook
ripol	686.00	NIST Webbook
ripol	714.00	NIST Webbook
ripol	718.00	NIST Webbook
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ripol	727.00	NIST Webbook
ripol	695.00	NIST Webbook
ripol	714.00	NIST Webbook
ripol	712.00	NIST Webbook
ripol	713.00	NIST Webbook
ripol	713.00	NIST Webbook
ripol	690.00	NIST Webbook
ripol	712.00	NIST Webbook
ripol	728.00	NIST Webbook
ripol	703.00	NIST Webbook
ripol	718.00	NIST Webbook
ripol	677.00	NIST Webbook
ripol	700.00	NIST Webbook
ripol	750.00	NIST Webbook
ripol	701.00	NIST Webbook
ripol	704.00	NIST Webbook
ripol	690.00	NIST Webbook
ripol	703.00	NIST Webbook

ripol	714.00		NIST Webbook
ripol	680.00		NIST Webbook
ripol	732.00		NIST Webbook
ripol	700.00		NIST Webbook
ripol	715.00		NIST Webbook
ripol	735.00		NIST Webbook
ripol	724.00		NIST Webbook
ripol	727.00		NIST Webbook
ripol	727.00		NIST Webbook
ripol	659.00		NIST Webbook
ripol	707.00		NIST Webbook
ripol	692.00		NIST Webbook
ripol	702.00		NIST Webbook
ripol	690.00		NIST Webbook
ripol	716.00		NIST Webbook
ripol	702.00		NIST Webbook
ripol	690.00		NIST Webbook
ripol	748.00		NIST Webbook
ripol	690.00		NIST Webbook
ripol	690.00		NIST Webbook
ripol	723.00		NIST Webbook
ripol	695.00		NIST Webbook
ripol	714.00		NIST Webbook
ripol	712.00		NIST Webbook
ripol	669.00		NIST Webbook
sl	117.30	J/mol×K	NIST Webbook
tb	294.15 ± 1.00	K	NIST Webbook
tb	294.00 ± 0.50	K	NIST Webbook
tb	293.35 ± 0.20	K	NIST Webbook
tb	294.15 ± 1.00	K	NIST Webbook
tb	294.15 ± 1.00	K	NIST Webbook
tb	294.15 ± 1.00	K	NIST Webbook
tb	293.95 ± 1.00	K	NIST Webbook
tb	293.95 ± 1.00	K	NIST Webbook
tb	294.20 ± 2.00	K	NIST Webbook
tb	293.75 ± 0.40	K	NIST Webbook
tb	293.90 ± 0.50	K	NIST Webbook
tb	293.35 ± 0.50	K	NIST Webbook
tb	293.85 ± 0.60	K	NIST Webbook
tb	308.87 ± 0.20	K	NIST Webbook
tb	293.65 ± 0.20	K	NIST Webbook
tb	294.95 ± 0.20	K	NIST Webbook
tb	293.00 ± 3.00	K	NIST Webbook
tb	293.95 ± 0.50	K	NIST Webbook

tb	294.65 ± 0.30	K	NIST Webbook
tb	293.90 ± 2.00	K	NIST Webbook
tb	294.15 ± 1.00	K	NIST Webbook
tb	295.70 ± 1.00	K	NIST Webbook
tb	293.90 ± 0.50	K	NIST Webbook
tb	293.55 ± 0.50	K	NIST Webbook
tb	294.00	K	NIST Webbook
tb	294.65 ± 1.00	K	NIST Webbook
tb	294.00	K	NIST Webbook
tb	293.84	K	Isobaric Vapor Liquid Equilibrium for Three Binary Systems of Acetaldehyde + Ethanol, Ethyl Acetate, 1-Butanol at 101.3 kPa
tb	293.20	K	KDB
tb	293.30	K	NIST Webbook
tc	454.70 ± 6.00	K	NIST Webbook
tc	461.00 ± 2.00	K	NIST Webbook
tc	466.00 ± 2.00	K	NIST Webbook
tc	466.00	K	KDB
tf	150.55 ± 0.30	K	NIST Webbook
tf	150.00	K	KDB
tf	154.70 ± 0.20	K	NIST Webbook
tf	148.60 ± 3.00	K	NIST Webbook
tf	149.90 ± 3.00	K	NIST Webbook
tf	149.70 ± 1.00	K	NIST Webbook
tf	148.60 ± 2.00	K	NIST Webbook
tf	149.70 ± 1.00	K	NIST Webbook
tf	152.50 ± 3.00	K	NIST Webbook
tf	152.60 ± 4.00	K	NIST Webbook
tf	149.70 ± 1.00	K	NIST Webbook
tf	149.70 ± 0.60	K	NIST Webbook
tf	152.00	K	NIST Webbook
tf	150.15 ± 1.00	K	NIST Webbook
tf	149.80 ± 0.60	K	NIST Webbook
tf	149.80 ± 0.60	K	NIST Webbook
tf	149.90 ± 1.00	K	NIST Webbook
vc	0.154	m3/kmol	KDB
zc	0.2213880		KDB
zra	0.24		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	67.45	J/mol×K	422.40	NIST Webbook
cpg	54.98	J/mol×K	298.10	NIST Webbook
cpg	58.03	J/mol×K	322.90	NIST Webbook
cpg	62.43	J/mol×K	372.70	NIST Webbook
cpl	96.21	J/mol×K	273.00	NIST Webbook
cpl	89.05	J/mol×K	298.15	NIST Webbook
dvisc	0.0017159	Pa×s	154.30	Joback Method
dvisc	0.0002044	Pa×s	293.82	Joback Method
dvisc	0.0009542	Pa×s	177.55	Joback Method
dvisc	0.0006079	Pa×s	200.81	Joback Method
dvisc	0.0004252	Pa×s	224.06	Joback Method
dvisc	0.0003181	Pa×s	247.31	Joback Method
dvisc	0.0002502	Pa×s	270.57	Joback Method
hfust	1.72	kJ/mol	242.90	NIST Webbook
hfust	2.31	kJ/mol	149.78	NIST Webbook
hfust	1.72	kJ/mol	242.90	NIST Webbook
hfust	2.31	kJ/mol	149.80	NIST Webbook
hvapt	26.00	kJ/mol	335.00	NIST Webbook
hvapt	25.76	kJ/mol	293.30	NIST Webbook
hvapt	25.73	kJ/mol	293.80	KDB
hvapt	26.30	kJ/mol	319.00	NIST Webbook
hvapt	27.00	kJ/mol	290.00	NIST Webbook
hvapt	27.60	kJ/mol	283.00	NIST Webbook
hvapt	25.70 ± 0.20	kJ/mol	294.00	NIST Webbook
rfi	1.33700		293.15	Vapor Liquid Equilibrium Data for 2,3-Pentanedione + (Acetaldehyde or Acetone) at (100, 150, and 200) kPa

rfi	1.33280		293.15	Geometric Structures of Associating Component Optimized toward Correlation and Prediction of Isobaric Vapor Liquid Equilibria for Binary and Ternary Mixtures of Ethanal, Ethanol, and Ethanoic Acid
rhol	778.00	kg/m3	293.00	KDB
sfust	15.42	J/mol×K	149.80	NIST Webbook
sfust	15.43	J/mol×K	149.78	NIST Webbook
sfust	7.06	J/mol×K	242.90	NIST Webbook
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48385e+01
Coeff. B	-2.70857e+03
Coeff. C	-2.88780e+01
Temperature range (K), min.	215.02
Temperature range (K), max.	466.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.30805e+02
Coeff. B	-7.24125e+03
Coeff. C	-1.82713e+01
Coeff. D	2.63363e-05
Temperature range (K), min.	150.15
Temperature range (K), max.	461.00

Sources

Infinite Dilution Activity Coefficients in Ethylene Glycol and Ethylene Carbonate:	https://www.doi.org/10.1021/je0102107
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Determination of Henry s Law Constants and Activity Coefficients at Infinite Dilution of Flavor Compounds in Water at 298 K with a Gas-Chromatographic Method:	https://www.doi.org/10.1021/je0495942
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Geometric Structures of Associating Component Optimized toward Correlation and Prediction of Isobaric Vapor Liquid Equilibria for Binary and Ternary Mixtures of Ethanal, Ethanol, and Ethanol Acetate:	https://www.doi.org/10.1021/je300810p
Measurement of activity coefficients at infinite dilution of organic solutes in KDB:	https://www.doi.org/10.1016/j.jct.2013.10.026
Ionic liquid 1-hexyl-1,4-diazo[2.2.2]bicyclooctanium bis(trifluoromethylsulfonyl)imide using gas-liquid chromatography:	https://www.cheric.org/files/research/kdb/mol/mol1232.mol
Quantitative NMR spectroscopy of binary liquid mixtures (aldehyde + alcohol): Part I: Acetaldehyde + (methanol or ethanol or 1-propanol):	https://www.doi.org/10.1016/j.jct.2013.03.022
Isobaric Vapor Liquid Equilibrium for Three Binary Systems of Acetaldehyde + Ethanol, Ethyl Acetate, 1-Butanol at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.7b00231
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1232
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1232
Vapor Liquid Equilibrium Data for 2,3-Pentanedione + (Acetaldehyde or Acetone) at (100, 150, and 200) kPa:	https://www.doi.org/10.1021/acs.jced.8b01196
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75070&Units=SI

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
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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