Acetic anhydride

Other names:	(CH3CO)2O
	Acetanhydride
	Acetic acid anhydride
	Acetic acid, 1,1'-anhydride
	Acetic acid, anhydride
	Acetic oxide
	Acetyl acetate
	Acetyl anhydride
	Acetyl ether
	Acetyl oxide
	Anhydrid kyseliny octove
	Anhydride acetique
	Anidride acetica
	Azijnzuuranhydride
	Essigsaeureanhydrid
	Ethanoic anhydrate
	Ethanoic anhydride
	Octowy bezwodnik
	UN 1715
Inchi:	InChI=1S/C4H6O3/c1-3(5)7-4(2)6/h1-2H3
InchiKey:	WFDIJRYMOXRFFG-UHFFFAOYSA-N
Formula:	C4H6O3
SMILES:	CC(=O)OC(C)=O
Mol. weight [g/mol]:	102.09
CAS:	108-24-7

Physical Properties

Property code	Value	Unit	Source
gf	-380.04	kJ/mol	Joback Method
hf	-483.27	kJ/mol	Joback Method
hfl	-625.00 ± 3.40	kJ/mol	NIST Webbook
hfus	10.50	kJ/mol	Joback Method
hvap	40.40	kJ/mol	Joback Method
ie	10.00	eV	NIST Webbook
log10ws	-0.13		Crippen Method
logp	0.096		Crippen Method
mcvol	76.230	ml/mol	McGowan Method

pc	4000.00 ± 200.00	kPa	NIST Webbook
pc	4680.00 ± 405.30	kPa	NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	706.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1227.00		NIST Webbook
ripol	1227.00		NIST Webbook
sg	389.95	J/mol×K	NIST Webbook
tb	410.00 ± 3.00	K	NIST Webbook
tb	412.65 ± 0.50	K	NIST Webbook
tb	412.70	K	NIST Webbook
tb	412.70	K	NIST Webbook
tb	412.65 ± 0.40	K	NIST Webbook
tb	412.15 ± 1.00	K	NIST Webbook
tb	413.15 ± 0.30	K	NIST Webbook
tb	412.60 ± 0.50	K	NIST Webbook
tb	413.00 ± 0.40	K	NIST Webbook
tb	412.55 ± 1.00	K	NIST Webbook
tb	403.55 ± 0.20	K	NIST Webbook
tc	569.00 ± 20.00	K	NIST Webbook
tc	606.00 ± 4.00	K	NIST Webbook
tf	199.11 ± 2.00	K	NIST Webbook
tf	200.00	K	NIST Webbook
tf	200.05 ± 0.40	K	NIST Webbook
tf	201.05 ± 0.50	K	NIST Webbook
tf	199.02 ± 0.07	K	NIST Webbook
tf	199.05 ± 1.00	K	NIST Webbook
tf	200.15 ± 0.30	K	NIST Webbook
tf	200.15 ± 0.40	K	NIST Webbook
tf	200.15 ± 1.00	K	NIST Webbook
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.35	J/mol×K	613.71	Joback Method
cpg	146.68	J/mol×K	453.18	Joback Method
cpg	140.13	J/mol×K	421.08	Joback Method

cpg	170.85	J/mol×K	581.60	Joback Method
cpg	165.13	J/mol×K	549.50	Joback Method
cpg	159.19	J/mol×K	517.39	Joback Method
cpg	153.04	J/mol×K	485.29	Joback Method
cpl	204.34	J/mol×K	333.15	Heat Capacities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
cpl	168.20	J/mol×K	303.20	NIST Webbook
cpl	200.73	J/mol×K	313.15	Heat Capacities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0006880	Pa×s	313.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0005480	Pa×s	333.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0006100	Pa×s	323.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0008880	Pa×s	293.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures

dvisc	0.0008290	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0007780	Pa×s	303.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0007290	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0006480	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0005800	Pa×s	328.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
dvisc	0.0005210	Pa×s	338.15	Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures
hvapt	44.20	kJ/mol	374.00	NIST Webbook
hvapt	45.50	kJ/mol	366.50	NIST Webbook
hvapt	47.60	kJ/mol	469.50	NIST Webbook
hvapt	43.30	kJ/mol	389.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	317.20	K	2.00	NIST Webbook
tbrp	317.00	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.70607e+02
Coeff. B	-1.12828e+04
Coeff. C	-2.37023e+01
Coeff. D	2.12043e-05
Temperature range (K), min.	200.15
Temperature range (K), max.	569.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol989.mol

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=989

Evaluation of Excess Molar Enthalpies for a Quaternary Mixture System of Acetic Anhydride, Ethanol, Acetic Acid, and Ethyl Acetate: https://www.doi.org/10.1021/je200595b

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

High pressure vapour liquid equilibria of the binary and some of the ternary and multicomponent mixtures of the carbon dioxide + acetic anhydride + ethyl acetate system: Experimental and modeling https://www.doi.org/10.1016/j.fluid.2006.04.011

Solubility Determination and Thermodynamic Modeling of Glutaric Acid in Ethanol + Ethyl Acetate Binary Solvent Mixtures at Different Temperatures https://www.doi.org/10.1021/acs.jced.8b00496

Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures https://www.doi.org/10.1021/je8003782

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

Measurement and correlation of solubility of D-camphor-10-sulfonic acid in pure solvents: https://www.doi.org/10.1016/j.fluid.2015.04.014

NIST Webbook http://webbook.nist.gov/cgi/cbook.cgi?ID=C108247&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Heat Capacities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures https://www.doi.org/10.1021/je9006579

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
ie:	Ionization energy
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
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume