1-Propen-2-ol, acetate

Other names:	1-Acetoxy-1-methylethylene
	1-Methylvinyl acetate
	1-Propen-2-ol, 2-acetate
	1-Propen-2-yl acetate
	1-methylvinyl ethanoate
	2-ACETOXYPROPENE
	2-Acetoxypropylene
	Acetic acid 1-methylethenyl ester
	Acetic acid isopropenyl ester
	ISOPROPENYL ACETATE
	METHYLVINYL ACETATE
	NSC 2197
	PROPEN-2-YL ACETATE
	UN 2403
	acetic acid, isopropenyl ester
	ethanoic acid, isopropenyl ester
	isopropenyl ethanoate
Inchi:	InChI=1S/C5H8O2/c1-4(2)7-5(3)6/h1H2,2-3H3
InchiKey:	HETCEOQFVDFGSY-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	C=C(C)OC(C)=O
Mol. weight [g/mol]:	100.12
CAS:	108-22-5

Physical Properties

Property code	Value	Unit	Source
gf	-163.41	kJ/mol	Joback Method
hf	-275.69	kJ/mol	Joback Method
hfl	-386.20 ± 0.96	kJ/mol	NIST Webbook
hfus	8.90	kJ/mol	Joback Method
hvap	35.29	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.083		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	644.00		NIST Webbook
rinpol	673.00		NIST Webbook

rinpol	609.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	608.00		NIST Webbook
tb	367.20	K	NIST Webbook
tb	370.00	K	NIST Webbook
tb	370.00 ± 2.00	K	NIST Webbook
tb	370.85	K	NIST Webbook
tc	572.77	K	Joback Method
tf	180.25	K	NIST Webbook
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.24	J/mol×K	510.73	Joback Method
cpg	186.04	J/mol×K	541.75	Joback Method
cpg	149.36	J/mol×K	386.65	Joback Method
cpg	157.23	J/mol×K	417.67	Joback Method
cpg	164.83	J/mol×K	448.69	Joback Method
cpg	172.17	J/mol×K	479.71	Joback Method
cpg	192.58	J/mol×K	572.77	Joback Method
rfi	1.40290		298.15	Isobaric Vapor Liquid Equilibria for Binary Systems of Acetone + Isopropenyl Acetate, 2-Butanone + Isopropenyl Acetate, and Isopropenyl Acetate + Acetylacetone at 101.3 kPa
rfi	1.40330		293.15	Isobaric Vapor-Liquid Equilibria for the Binary Systems of Acetic Acid + Isopropenyl Acetate, Acetic Acid + Acetylacetone, and Water + Acetylacetone

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54161e+01
Coeff. B	-3.49774e+03
Coeff. C	-4.32180e+01
Temperature range (K), min.	274.42
Temperature range (K), max.	389.37

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.62473e+01
Coeff. B	-4.31771e+03
Coeff. C	6.24722e-03
Coeff. D	-8.51795e-09
Temperature range (K), min.	332.15
Temperature range (K), max.	370.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1170
Liquid-liquid equilibrium for the ternary system isopropenyl acetate + water + acetic acid at 298.2 K, 313.2 K, 323.2 K and 333.2 K:	https://www.doi.org/10.1016/j.fluid.2011.09.001
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1170
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isobaric vapor-liquid liquid equilibrium for isopropenyl acetate + water + acetic acid at 101 kPa:	https://www.doi.org/10.1016/j.fluid.2011.10.025
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108225&Units=SI
Isobaric Vapor Liquid Equilibria for Binary Systems of Acetone + Isopropenyl Acetate, 2-Butanone + Isopropenyl Acetate, and Isopropenyl Acetate + Acetylacetone at 101.3 kPa:	https://www.doi.org/10.1021/je700605t
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric Vapor-Liquid Equilibria for the Binary Systems of Acetic Acid + Isopropenyl Acetate, Acetic Acid + Acetylacetone, and Water + Acetylacetone:	https://www.doi.org/10.1021/je800345j
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume