Acetic acid, 1,1-dimethylethyl ester

Other names:	1,1-Dimethylethyl acetate
	1,1-dimethylethyl ethanoate
	Acetic acid t-butyl ester
	Acetic acid, tert-butyl ester
	CH3C(O)OC(CH3)3
	NSC 59719
	TERT-BUTYL ESTER ACETIC ACID
	TERT-BUTYL ETHANOATE
	TLA
	Texaco lead appreciator
	t-Butyl acetate
	tert-Butyl acetate
Inchi:	InChI=1S/C6H12O2/c1-5(7)8-6(2,3)4/h1-4H3
InchiKey:	WMOVHXAZOJBABW-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC(=O)OC(C)(C)C
Mol. weight [g/mol]:	116.16
CAS:	540-88-5

Physical Properties

Property code	Value	Unit	Source
chl	-3521.50 ± 1.30	kJ/mol	NIST Webbook
gf	-231.44	kJ/mol	Joback Method
hf	-516.50 ± 1.30	kJ/mol	NIST Webbook
hfl	-554.50 ± 1.30	kJ/mol	NIST Webbook
hfus	6.67	kJ/mol	Joback Method
hvap	38.00 ± 0.20	kJ/mol	NIST Webbook
hvap	38.00 ± 0.20	kJ/mol	NIST Webbook
hvap	38.00	kJ/mol	NIST Webbook
hvap	38.03 ± 0.21	kJ/mol	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.348		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3040.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method

rinpol	687.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	701.40		NIST Webbook
ripol	912.50		NIST Webbook
ripol	893.00		NIST Webbook
ripol	878.00		NIST Webbook
ripol	912.50		NIST Webbook
ripol	845.00		NIST Webbook
ripol	888.00		NIST Webbook
ripol	893.00		NIST Webbook
ripol	893.00		NIST Webbook
tb	371.05	K	Isobaric Vapor-Liquid Equilibrium for Binary and Ternary Systems of tert-Butanol + tert-Butyl Acetate + Chlorobenzene at 101.33 kPa
tb	371.00 ± 0.40	K	NIST Webbook
tb	369.20 ± 2.00	K	NIST Webbook
tb	369.00	K	NIST Webbook
tb	370.70	K	NIST Webbook
tb	369.15	K	Isobaric Vapor-Liquid Equilibrium for the Binary Systems of 1,2-Dichloroethane + sec-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate at 101.3 kPa
tb	369.00 ± 3.00	K	NIST Webbook
tc	599.15	K	Joback Method
tf	231.96	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.96	J/mol×K	409.74	Joback Method
cpg	261.33	J/mol×K	599.15	Joback Method
cpg	252.62	J/mol×K	567.58	Joback Method
cpg	243.45	J/mol×K	536.01	Joback Method
cpg	233.81	J/mol×K	504.44	Joback Method
cpg	223.69	J/mol×K	472.88	Joback Method
cpg	213.08	J/mol×K	441.31	Joback Method
cpl	231.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0022923	Pa×s	261.59	Joback Method
dvisc	0.0012870	Pa×s	291.22	Joback Method
dvisc	0.0008038	Pa×s	320.85	Joback Method
dvisc	0.0005436	Pa×s	350.48	Joback Method
dvisc	0.0003908	Pa×s	380.11	Joback Method
dvisc	0.0002947	Pa×s	409.74	Joback Method
dvisc	0.0047319	Pa×s	231.96	Joback Method
hvapt	36.70	kJ/mol	340.00	NIST Webbook
pvap	101.33	kPa	371.05	Isobaric Vapor-Liquid Equilibrium for Binary and Ternary Systems of tert-Butanol + tert-Butyl Acetate + Chlorobenzene at 101.33 kPa
pvap	101.30	kPa	369.15	Isobaric Vapor-Liquid Equilibrium for the Binary Systems of 1,2-Dichloroethane + sec-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate at 101.3 kPa
rfi	1.38400		298.15	Isobaric vapor-liquid equilibria for the binary systems isobutyl alcohol + isobutyl acetate and tert-butyl alcohol + tert-butyl acetate at 20 and 101.3 kPa

speedsl	1049.00	m/s	308.15	Densities, Sound Speed, and IR Studies of (Methanol + 1-Acetoxybutane) and (Methanol + 1,1-Dimethylethyl Ester) at (298.15, 303.15, 308.15, and 313.15) K	
speedsl	1078.00	m/s	303.15	Densities, Sound Speed, and IR Studies of (Methanol + 1-Acetoxybutane) and (Methanol + 1,1-Dimethylethyl Ester) at (298.15, 303.15, 308.15, and 313.15) K	
speedsl	1091.00	m/s	298.15	Densities, Sound Speed, and IR Studies of (Methanol + 1-Acetoxybutane) and (Methanol + 1,1-Dimethylethyl Ester) at (298.15, 303.15, 308.15, and 313.15) K	
speedsl	1040.00	m/s	313.15	Densities, Sound Speed, and IR Studies of (Methanol + 1-Acetoxybutane) and (Methanol + 1,1-Dimethylethyl Ester) at (298.15, 303.15, 308.15, and 313.15) K	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41156e+01
Coeff. B	-3.02399e+03
Coeff. C	-5.22940e+01
Temperature range (K), min.	270.98
Temperature range (K), max.	395.77

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.57842e+01
Coeff. B	-7.25311e+03
Coeff. C	-1.05853e+01
Coeff. D	7.65791e-06
Temperature range (K), min.	283.15
Temperature range (K), max.	545.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C540885&Units=SI
Critical Point and Vapor Pressure Measurements for 17 Compounds by a McGowan Method:	https://www.doi.org/10.1021/je060269j
Low Residence Time Flow Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Liquid-Liquid Equilibria for the Acetic Acid + Water + Amyl Acetate and Acetic Acid + Water + 2-Methyl-1-Ethyl Acetate, Ternary Systems:	https://www.doi.org/10.1021/je700181d
Densities, viscosities, speed of sound, and IR spectroscopic studies of binary mixtures of tert-butyl acetate with benzene, methylbenzene, and ethylbenzene at T = (298.15 and 308.15) K:	https://www.doi.org/10.1016/j.jct.2011.04.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Isobaric vapor-liquid equilibria for the binary systems isobutyl alcohol + isobutyl acetate and tert-butyl alcohol + tert-butyl acetate at 20 and 101.3 kPa:	https://www.doi.org/10.1016/j.fluid.2004.10.022
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1082
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and limiting activity coefficient of simvastatin in different organic solvents:	https://www.doi.org/10.1016/j.fluid.2009.03.006
Isobaric Vapor-Liquid Equilibrium for the Binary Systems of 1,2-Dichloroethane + sec-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.8b00434
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 butyl acetate:	https://www.doi.org/10.1016/j.tca.2016.04.001
Densities, Sound Speed, and Refractive Index Data for Binary Mixtures of Methanol + 1-Acetoxybutane and 1,3-Dichloro-2-propanol with Ethyl Acetate and Propyl Acetate at (298.15 and 308.15) K:	https://www.doi.org/10.1021/je900442b
Isobaric Vapor–Liquid Equilibrium for Binary Systems of Propyl Acetate + Butyl Acetate + Chlorobenzene at 101.33 kPa:	https://www.doi.org/10.1021/acs.jced.7b01021
Solubility of Lovastatin in Ethyl Acetate, Propyl Acetate, Isopropyl Acetate, Butyl Acetate, sec-Butyl Acetate, Isobutyl Acetate, tert-Butyl Acetate, and 2-Butanone, between (285 and 313) K:	https://www.cheric.org/files/research/kdb/mol/mol1082.mol
	https://www.doi.org/10.1021/je800120p

Legend

chl:	Standard liquid enthalpy of combustion
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
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
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume