Acetic acid, pentyl ester

Other names:	1-Acetoxypentane
	1-PENTYL ACETATE
	1-Pentanol acetate
	AMYL ACETIC ESTER
	Acetate d'amyle
	Acetic acid n-amyl ester
	Acetic acid, amyl ester
	Acetic acid, n-pentyl ester
	Amyl acetate
	Amyl acetic ether
	Amylazetat
	Amylester kyseliny octove
	Banana oil
	Birnenoel
	N-AMYL ACETATE
	N-PENTYL ACETATE
	NSC 7923
	Octan amylu
	Pear oil
	Pent-acetate
	Pent-acetate 28
	Pentyl acetate
	Pentyl ester of acetic acid
	Primary amyl acetate
	acetic acid, n-amyl ester
	ethanoic acid, pentyl ester
	n-Pentyl ethanoate
	pentyl ethanoate
Inchi:	InChI=1S/C7H14O2/c1-3-4-5-6-9-7(2)8/h3-6H2,1-2H3
InchiKey:	PGMYKACGEOXYJE-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCCCCOC(C)=O
Mol. weight [g/mol]:	130.18
CAS:	628-63-7

Physical Properties

Property code	Value	Unit	Source

chl	-4372.13	kJ/mol	NIST Webbook
gf	-225.86	kJ/mol	Joback Method
hf	-432.61	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	48.60 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.89		Aqueous Solubility Prediction Method
log10ws	-1.89		Estimated Solubility Method
logp	1.740		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	2685.00 ± 150.00	kPa	NIST Webbook
pc	2770.00 ± 20.00	kPa	NIST Webbook
rhoc	277.42 ± 11.98	kg/m3	NIST Webbook
rinpol	896.50		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	914.00		NIST Webbook

rinpol	893.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	928.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	917.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	918.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	912.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	913.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	905.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	915.00	NIST Webbook
rinpol	910.00	NIST Webbook
rinpol	859.00	NIST Webbook
rinpol	897.00	NIST Webbook
rinpol	911.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	897.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	916.00	NIST Webbook
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rinpol	912.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	918.00	NIST Webbook

rinpol	895.00	NIST Webbook
rinpol	891.00	NIST Webbook
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rinpol	892.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	912.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	907.60	NIST Webbook
rinpol	909.30	NIST Webbook
rinpol	910.30	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	908.68	NIST Webbook
rinpol	887.63	NIST Webbook
rinpol	896.40	NIST Webbook
rinpol	859.00	NIST Webbook
rinpol	898.00	NIST Webbook
ripol	1175.00	NIST Webbook
ripol	1195.00	NIST Webbook
ripol	1182.00	NIST Webbook
ripol	1212.00	NIST Webbook
ripol	1168.00	NIST Webbook
ripol	1182.00	NIST Webbook
ripol	1177.00	NIST Webbook
ripol	1175.00	NIST Webbook
ripol	1177.00	NIST Webbook
ripol	1196.00	NIST Webbook
ripol	1170.00	NIST Webbook
ripol	1160.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1152.00	NIST Webbook
ripol	1176.00	NIST Webbook
ripol	1193.00	NIST Webbook
ripol	1182.00	NIST Webbook
ripol	1169.00	NIST Webbook
ripol	1161.00	NIST Webbook

ripol	1167.00	NIST Webbook
ripol	1176.00	NIST Webbook
ripol	1179.00	NIST Webbook
ripol	1181.00	NIST Webbook
ripol	1167.00	NIST Webbook
ripol	1152.00	NIST Webbook
ripol	1169.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1176.00	NIST Webbook
ripol	1204.00	NIST Webbook
ripol	1162.00	NIST Webbook
ripol	1192.00	NIST Webbook
ripol	1169.00	NIST Webbook
ripol	1150.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1185.00	NIST Webbook
ripol	1194.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1173.00	NIST Webbook
ripol	1172.00	NIST Webbook
ripol	1167.00	NIST Webbook
ripol	1177.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1174.00	NIST Webbook
ripol	1174.00	NIST Webbook
ripol	1222.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1159.00	NIST Webbook
ripol	1169.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1174.00	NIST Webbook
ripol	1185.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1177.00	NIST Webbook
ripol	1194.00	NIST Webbook
ripol	1194.00	NIST Webbook
ripol	1176.00	NIST Webbook

ripol	1161.00		NIST Webbook
ripol	1159.00		NIST Webbook
tb	422.25	K	Quaternary phase equilibrium of water-carboxylic acid mixture (formic-propionic acid or acetic-propionic acid)-solvent liquid systems at 298.15 K
tc	599.90 ± 0.60	K	NIST Webbook
tc	600.00 ± 2.00	K	NIST Webbook
tf	202.35 ± 0.30	K	NIST Webbook
tf	182.88	K	Aqueous Solubility Prediction Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.73	J/mol×K	612.24	Joback Method
cpg	249.76	J/mol×K	465.25	Joback Method
cpg	260.50	J/mol×K	494.65	Joback Method
cpg	270.86	J/mol×K	524.04	Joback Method
cpg	280.85	J/mol×K	553.44	Joback Method
cpg	290.48	J/mol×K	582.84	Joback Method
cpg	238.65	J/mol×K	435.85	Joback Method
cpl	276.10	J/mol×K	304.00	NIST Webbook
dvisc	0.0004549	Pa×s	370.84	Joback Method
dvisc	0.0006434	Pa×s	338.33	Joback Method
dvisc	0.0009795	Pa×s	305.82	Joback Method
dvisc	0.0016480	Pa×s	273.32	Joback Method
dvisc	0.0031909	Pa×s	240.81	Joback Method
dvisc	0.0002656	Pa×s	435.85	Joback Method
dvisc	0.0003401	Pa×s	403.34	Joback Method
hvapt	43.20	kJ/mol	376.00	NIST Webbook
pvap	0.11	kPa	278.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.34	kPa	293.30	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.48	kPa	298.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.66	kPa	303.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.81	kPa	306.70	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.90	kPa	308.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	1.03	kPa	310.60	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	1.22	kPa	313.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.14	kPa	280.80	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	53.33	kPa	400.72	Isobaric Vapor-Liquid Equilibria of the Ternary System Toluene + Ethylbenzene + Amyl Acetate
pvap	79.99	kPa	414.20	Isobaric Vapor-Liquid Equilibria of the Ternary System Toluene + Ethylbenzene + Amyl Acetate
pvap	0.24	kPa	288.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.09	kPa	274.20	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.09	kPa	274.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.10	kPa	275.60	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.10	kPa	275.60	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.17	kPa	283.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	26.66	kPa	380.05	Isobaric Vapor-Liquid Equilibria of the Ternary System Toluene + Ethylbenzene + Amyl Acetate
rfi	1.40050		298.15	Isobaric Vapor-Liquid Equilibrium for Binary Mixtures of 3-Methyl-1-butanol + 3-Methyl-1-butyl Ethanoate and 1-Pentanol + Pentyl Ethanoate at 101.3 kPa
rfi	1.40260		293.15	Phase equilibria of water + 1-propanol + solvent (n-amyl acetate, cyclohexanol, and cyclohexyl acetate) at T = 298.2K
rfi	1.39100		318.15	Thermodynamic properties of (an ester + an alkane). XVI. Experimental HEm and V Em values and a new correlation method for (an alkyl ethanoate + an n-alkane) at 318.15 K

rfi	1.39910		298.20	Experimental and correlated liquid-liquid equilibrium data for water-phosphoric acid-ester
rfi	1.39610		303.15	Densities, speeds of sound, isentropic compressibilities, refractive indexes, and viscosities of tetrahydrofuran with haloalkane or alkyl ethanoate at T = 303.15 K
rfi	1.39990		298.15	Isobaric Vapor-Liquid Equilibria of Binary Mixtures of Diethyl Carbonate with Methyl Acetate, n-Propyl Acetate, or Amyl Acetate at 100.17 kPa
rfi	1.40270		293.13	Isobaric Vapor-Liquid Equilibria of the Ternary System Pentan-1-ol + Pentyl Acetate + Nonane
rfi	1.40210		293.15	Isobaric Vapor-Liquid Equilibria for Water + Acetic Acid + (n-Pentyl Acetate or Isopropyl Acetate)
rhol	855.36	kg/m3	313.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)
rhol	860.58	kg/m3	308.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)

rhol	865.78	kg/m3	303.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)
rhol	871.32	kg/m3	298.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)
rhol	876.25	kg/m3	293.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)
rhol	870.17	kg/m3	298.15	Experimental and theoretical study of surface tension of binary mixtures of (n-alkyl acetates + heptane, benzene, and toluene)
rhol	870.17	kg/m3	298.15	Surface Tension and Surface Properties of Binary Mixtures of 1,4-Dioxane or N,N-Dimethyl Formamide with n-Alkyl Acetates

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53552e+01
Coeff. B	-3.88429e+03
Coeff. C	-5.82300e+01
Temperature range (K), min.	316.02
Temperature range (K), max.	444.97

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.62684e+01
Coeff. B	-8.63027e+03
Coeff. C	-1.02643e+01
Coeff. D	4.74624e-06
Temperature range (K), min.	202.35
Temperature range (K), max.	598.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	871.4
298.15	1000.00	871.9
298.15	2000.00	872.7
298.15	2700.00	873.3
298.15	3000.00	873.5
298.15	5000.00	875.3
298.15	10000.00	879.1
298.15	15000.00	882.7
298.15	20000.00	886.2
298.15	25000.00	889.6
298.15	30000.00	893.6
298.15	35000.00	897.9
303.15	100.00	866.5
303.15	1000.00	867.1
303.15	2000.00	867.9
303.15	2700.00	868.5
303.15	3000.00	868.7
303.15	5000.00	870.5
303.15	10000.00	874.4
303.15	15000.00	878.1
303.15	20000.00	881.6
303.15	25000.00	885.1
303.15	30000.00	889.4
303.15	35000.00	893.8
308.15	100.00	861.6

308.15	1000.00	862.2
308.15	2000.00	863.1
308.15	2700.00	863.7
308.15	3000.00	863.9
308.15	5000.00	865.8
308.15	10000.00	869.8
308.15	15000.00	873.6
308.15	20000.00	877.3
308.15	25000.00	880.8
308.15	30000.00	885.2
308.15	35000.00	889.7
313.15	100.00	856.7
313.15	1000.00	857.4
313.15	2000.00	858.3
313.15	2700.00	858.9
313.15	3000.00	859.2
313.15	5000.00	861.0
313.15	10000.00	865.2
313.15	15000.00	869.0
313.15	20000.00	872.8
313.15	25000.00	876.4
313.15	30000.00	880.9
313.15	35000.00	885.5
318.15	100.00	851.9
318.15	1000.00	852.6
318.15	2000.00	853.5
318.15	2700.00	854.2
318.15	3000.00	854.4
318.15	5000.00	856.4
318.15	10000.00	860.7
318.15	15000.00	864.7
318.15	20000.00	868.5
318.15	25000.00	872.3
318.15	30000.00	876.9
318.15	35000.00	881.7
323.15	100.00	847.1
323.15	1000.00	847.7
323.15	2000.00	848.7
323.15	2700.00	849.3
323.15	3000.00	849.6
323.15	5000.00	851.7
323.15	10000.00	856.1
323.15	15000.00	860.2
323.15	20000.00	864.2

323.15	25000.00	868.1
323.15	30000.00	872.8
323.15	35000.00	877.6
328.15	100.00	842.3
328.15	1000.00	843.2
328.15	2000.00	844.4
328.15	2700.00	845.2
328.15	3000.00	845.5
328.15	5000.00	847.1
328.15	10000.00	851.6
328.15	15000.00	855.9
328.15	20000.00	860.0
328.15	25000.00	864.1
328.15	30000.00	869.0
328.15	35000.00	874.0
333.15	100.00	837.8
333.15	1000.00	838.7
333.15	2000.00	839.8
333.15	2700.00	840.5
333.15	3000.00	840.8
333.15	5000.00	842.7
333.15	10000.00	847.4
333.15	15000.00	851.8
333.15	20000.00	856.0
333.15	25000.00	860.1
333.15	30000.00	865.1
333.15	35000.00	870.2
338.15	100.00	832.9
338.15	1000.00	834.0
338.15	2000.00	835.1
338.15	2700.00	835.8
338.15	3000.00	836.1
338.15	5000.00	838.1
338.15	10000.00	842.9
338.15	15000.00	847.5
338.15	20000.00	851.9
338.15	25000.00	856.2
338.15	30000.00	861.3
338.15	35000.00	866.5
343.15	100.00	828.3
343.15	1000.00	829.3
343.15	2000.00	830.4
343.15	2700.00	831.2
343.15	3000.00	831.5

343.15	5000.00	833.5
343.15	10000.00	838.5
343.15	15000.00	843.2
343.15	20000.00	847.7
343.15	25000.00	852.1
343.15	30000.00	857.3
343.15	35000.00	862.7
348.15	100.00	823.2
348.15	1000.00	824.6
348.15	2000.00	825.7
348.15	2700.00	826.5
348.15	3000.00	826.9
348.15	5000.00	828.8
348.15	10000.00	834.0
348.15	15000.00	838.9
348.15	20000.00	843.5
348.15	25000.00	847.9
348.15	30000.00	853.3
348.15	35000.00	858.8
353.15	100.00	818.7
353.15	1000.00	819.9
353.15	2000.00	821.1
353.15	2700.00	821.9
353.15	3000.00	822.3
353.15	5000.00	824.4
353.15	10000.00	829.8
353.15	15000.00	835.0
353.15	20000.00	839.7
353.15	25000.00	844.3
353.15	30000.00	849.8
353.15	35000.00	855.4
358.15	100.00	811.3
358.15	1000.00	812.2
358.15	2000.00	813.4
358.15	2700.00	814.1
358.15	3000.00	814.5
358.15	5000.00	816.9
358.15	10000.00	822.5
358.15	15000.00	827.7
358.15	20000.00	832.5
358.15	25000.00	838.0
358.15	30000.00	843.9
358.15	35000.00	849.7
363.15	100.00	806.3

363.15	1000.00	807.4
363.15	2000.00	808.7
363.15	2700.00	809.6
363.15	3000.00	809.9
363.15	5000.00	812.4
363.15	10000.00	818.1
363.15	15000.00	823.4
363.15	20000.00	828.3
363.15	25000.00	833.9
363.15	30000.00	839.9
363.15	35000.00	845.6
368.15	100.00	801.2
368.15	1000.00	802.3
368.15	2000.00	803.7
368.15	2700.00	804.6
368.15	3000.00	805.0
368.15	5000.00	807.5
368.15	10000.00	813.4
368.15	15000.00	818.8
368.15	20000.00	824.0
368.15	25000.00	829.8
368.15	30000.00	835.9
368.15	35000.00	841.4
373.15	100.00	795.5
373.15	1000.00	796.4
373.15	2000.00	797.7
373.15	2700.00	799.5
373.15	3000.00	799.0
373.15	5000.00	802.5
373.15	10000.00	808.2
373.15	15000.00	813.9
373.15	20000.00	819.8
373.15	25000.00	826.3
373.15	30000.00	831.3
378.15	100.00	790.4
378.15	1000.00	791.6
378.15	2000.00	793.1
378.15	2700.00	794.0
378.15	3000.00	794.4
378.15	5000.00	797.1
378.15	10000.00	803.5
383.15	100.00	786.8
383.15	1000.00	788.1
383.15	2000.00	789.6

383.15	2700.00	790.7
383.15	3000.00	791.1
383.15	5000.00	793.9
383.15	10000.00	800.5
383.15	15000.00	806.6
383.15	20000.00	811.7
383.15	25000.00	816.5
383.15	30000.00	824.0
383.15	35000.00	830.0
388.15	100.00	781.9
388.15	1000.00	783.4
388.15	2000.00	785.0
388.15	2700.00	786.0
388.15	3000.00	786.5
388.15	5000.00	789.4
388.15	10000.00	796.3
388.15	15000.00	802.5
388.15	20000.00	808.1
388.15	25000.00	813.7
388.15	30000.00	819.7
388.15	35000.00	826.2
393.15	100.00	777.2
393.15	1000.00	778.7
393.15	2000.00	780.3
393.15	2700.00	781.4
393.15	3000.00	781.9
393.15	5000.00	784.9
393.15	10000.00	791.9
393.15	15000.00	798.4
393.15	20000.00	803.9
393.15	25000.00	809.7
393.15	30000.00	815.7
393.15	35000.00	822.2

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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
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
nfpaf:	NFPA Fire 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume