

2-Pentanone

Other names:	ETHYL ACETONE
	MPK
	Methyl n-propyl ketone
	Methyl propyl ketone
	Metylopropyloketon
	NSC 5350
	Pentan-2-one
	Pentanone-2
	Propyl methyl ketone
	UN 1249
	n-C3H7COCH3
	n-Propyl methyl ketone
	InChI=1S/C5H10O/c1-3-4-5(2)6/h3-4H2,1-2H3
Inchi:	
InchiKey:	XNLICIUVMPYHGG-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CCCC(C)=O
Mol. weight [g/mol]:	86.13
CAS:	107-87-9

Physical Properties

Property code	Value	Unit	Source
af	0.3460		KDB
affp	832.70	kJ/mol	NIST Webbook
basg	800.90	kJ/mol	NIST Webbook
chg	-3156.00	kJ/mol	NIST Webbook
chl	-3099.40 ± 0.80	kJ/mol	NIST Webbook
dm	2.50	debye	KDB
gf	-137.20	kJ/mol	KDB
hf	-259.10 ± 1.10	kJ/mol	NIST Webbook
hf	-258.80	kJ/mol	KDB
hfl	-297.30 ± 1.10	kJ/mol	NIST Webbook
hfus	10.30	kJ/mol	Joback Method
hvap	38.43	kJ/mol	NIST Webbook
hvap	38.46	kJ/mol	NIST Webbook
hvap	38.30 ± 0.30	kJ/mol	NIST Webbook
hvap	38.40	kJ/mol	NIST Webbook
hvap	38.40	kJ/mol	NIST Webbook

ie	9.37 ± 0.02	eV	NIST Webbook
ie	9.39 ± 0.02	eV	NIST Webbook
ie	9.38 ± 0.01	eV	NIST Webbook
ie	9.28 ± 0.02	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
ie	9.40 ± 0.01	eV	NIST Webbook
ie	9.38 ± 0.06	eV	NIST Webbook
ie	9.47 ± 0.03	eV	NIST Webbook
log10ws	-0.19		Estimated Solubility Method
log10ws	-0.19		Aqueous Solubility Prediction Method
logp	1.375		Crippen Method
mccvol	82.880	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	3694.00 ± 20.00	kPa	NIST Webbook
pc	3890.00 ± 48.30	kPa	NIST Webbook
pc	3694.00	kPa	KDB
rhoc	285.96 ± 7.75	kg/m3	NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	665.69		NIST Webbook
rinpol	666.90		NIST Webbook
rinpol	672.20		NIST Webbook
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sl	274.10	J/mol×K	NIST Webbook
sl	272.42	J/mol×K	NIST Webbook
tb	375.50 ± 0.30	K	NIST Webbook
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tb	376.15 ± 2.00	K	NIST Webbook
tb	375.65 ± 3.00	K	NIST Webbook
tb	375.41	K	KDB

tb	375.36	K	Measurement of Isobaric Vapor - Liquid Equilibria of Dimethyl Carbonate with Acetone, 2-Butanone and 2-Pentanone at 101.3 kPa and Density and Speed of Sound at 298.15 K
tb	375.20	K	NIST Webbook
tb	375.40	K	NIST Webbook
tb	375.45 ± 0.30	K	NIST Webbook
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tt	196.31 ± 0.04	K	NIST Webbook
tt	196.29 ± 0.07	K	NIST Webbook
vc	0.301	m3/kmol	KDB
zc	0.2383430		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.62 ± 0.45	J/mol×K	394.00	NIST Webbook
cpg	156.40 ± 0.47	J/mol×K	414.00	NIST Webbook
cpg	162.00 ± 0.49	J/mol×K	434.00	NIST Webbook
cpg	167.15 ± 0.50	J/mol×K	454.00	NIST Webbook
cpg	142.97 ± 0.43	J/mol×K	369.00	NIST Webbook
cpl	185.40	J/mol×K	298.15	NIST Webbook
cpl	184.20	J/mol×K	298.15	NIST Webbook
cpl	184.30	J/mol×K	298.15	NIST Webbook
cpl	185.10	J/mol×K	298.15	NIST Webbook
cpl	184.35	J/mol×K	298.15	NIST Webbook

dvisc	0.0004440	Pa×s	303.15	Dynamic Viscosities of the Binary Systems Cyclohexane and Cyclopentane with Acetone, Butanone, or 2-Pentanone at Three Temperatures T) (293.15, 298.15, and 303.15) K
dvisc	0.0004690	Pa×s	298.15	Dynamic Viscosities of the Binary Systems Cyclohexane and Cyclopentane with Acetone, Butanone, or 2-Pentanone at Three Temperatures T) (293.15, 298.15, and 303.15) K
dvisc	0.0004440	Pa×s	303.15	Physical properties of the binary systems methylcyclopentane with ketones (acetone, butanone and 2-pentanone) at T = (293.15, 298.15, and 303.15) K. New UNIFAC-VISCO interaction parameters
dvisc	0.0004690	Pa×s	298.15	Physical properties of the binary systems methylcyclopentane with ketones (acetone, butanone and 2-pentanone) at T = (293.15, 298.15, and 303.15) K. New UNIFAC-VISCO interaction parameters
dvisc	0.0004960	Pa×s	293.15	Dynamic Viscosities of the Binary Systems Cyclohexane and Cyclopentane with Acetone, Butanone, or 2-Pentanone at Three Temperatures T) (293.15, 298.15, and 303.15) K

dvisc	0.0004960	Paxs	293.15	Physical properties of the binary systems methylcyclopentane with ketones (acetone, butanone and 2-pentanone) at T = (293.15, 298.15, and 303.15) K. New UNIFAC-VISCO interaction parameters
hfust	10.63	kJ/mol	196.30	NIST Webbook
hfust	2.09	kJ/mol	110.00	NIST Webbook
hfust	10.62	kJ/mol	196.35	NIST Webbook
hvapt	36.10	kJ/mol	379.00	NIST Webbook
hvapt	33.44	kJ/mol	375.40	NIST Webbook
hvapt	33.47	kJ/mol	375.40	KDB
hvapt	33.30	kJ/mol	524.00	NIST Webbook
hvapt	36.50	kJ/mol	357.00	NIST Webbook
hvapt	36.10 ± 0.10	kJ/mol	335.00	NIST Webbook
hvapt	34.40 ± 0.10	kJ/mol	360.00	NIST Webbook
hvapt	32.20 ± 0.10	kJ/mol	394.00	NIST Webbook
hvapt	33.40 ± 0.10	kJ/mol	375.00	NIST Webbook
hvapt	32.80 ± 0.10	kJ/mol	386.00	NIST Webbook
hvapt	39.50	kJ/mol	320.50	NIST Webbook
hvapt	33.70	kJ/mol	458.50	NIST Webbook
rfi	1.38823		298.15	Properties of ionic liquid HMIMPF6 with carbonates, ketones and alkyl acetates
rfi	1.38810		298.15	Phase Equilibria in the Binary and Ternary Systems Composed of Diethyl ketone, 2-Pentanone and 3-Pentanol at 101.3 kPa
rfi	1.38930		293.15	Solubility Data for Roflumilast and Maraviroc in Various Solvents between T = (278.2-323.2) K

rfi	1.38920		293.15	Solid-Liquid Equilibrium Measurements for Posaconazole and Voriconazole in Several Solvents between T = 278.2 and 323.2 K Using Differential Thermal Analysis/Thermal Gravimetric Analysis
rfi	1.38930		293.15	Isothermal Vapor-Liquid Equilibrium Measurements for the Pentan-2-one + Propan-1-ol/Butan-1-ol System within 342-363 K
rfi	1.39060		293.15	Isothermal Vapor-Liquid Equilibrium for the 2-Pentanone (MPK) + 2-Methyl Propan-1-ol Binary Mixture
rfi	1.38830		298.15	Excess molar volumes and ultrasonic studies of N-methyl-2-pyrrolidone with ketones at T = 303.15 K
rhol	781.83	kg/m3	318.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhol	802.46	kg/m3	298.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K

rhoI	797.53	kg/m3	303.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K
rhoI	792.52	kg/m3	308.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K
rhoI	787.44	kg/m3	313.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K
rhoI	807.47	kg/m3	293.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K
rhoI	801.52	kg/m3	298.15	Thermodynamics of Ketone + Amine Mixtures. Part VIII. Molar Excess Enthalpies at 298.15 K for n-Alkanone + Aniline or + N-Methylaniline Systems

rhoI	762.27	kg/m3	338.15	Density, Speed of Sound, and Refractive Index Measurements for Binary Mixtures of Pentan-2-one with Propan-2-ol and Butan-2-ol
rhoI	791.66	kg/m3	308.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhoI	782.44	kg/m3	318.15	Density, Speed of Sound, and Refractive Index Measurements for Binary Mixtures of Pentan-2-one with Propan-2-ol and Butan-2-ol
rhoI	792.32	kg/m3	308.15	Density, Speed of Sound, and Refractive Index Measurements for Binary Mixtures of Pentan-2-one with Propan-2-ol and Butan-2-ol
rhoI	802.09	kg/m3	298.15	Density, Speed of Sound, and Refractive Index Measurements for Binary Mixtures of Pentan-2-one with Propan-2-ol and Butan-2-ol
rhoI	801.52	kg/m3	298.15	Thermodynamics of ketone + amine mixtures. Part IX. Excess molar enthalpies at 298.15K for dipropylamine, or dibutylamine + 2-alkanone systems and modeling of linear or aromatic amine + 2-alkanone mixtures in terms of DISQUAC and ERAS

rhoI	811.06	kg/m3	288.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhoI	787.16	kg/m3	313.15	Excess molar volumes of (1-chlorobutane +heptane + 2-butanone or 2-pentanone) at 288.15 , 303.15 and 313.15 K . Measurements and correlations.
rhoI	796.96	kg/m3	303.15	Excess molar volumes of (1-chlorobutane +heptane + 2-butanone or 2-pentanone) at 288.15 , 303.15 and 313.15 K . Measurements and correlations.
rhoI	811.49	kg/m3	288.15	Excess molar volumes of (1-chlorobutane +heptane + 2-butanone or 2-pentanone) at 288.15 , 303.15 and 313.15 K . Measurements and correlations.
rhoI	796.73	kg/m3	303.15	Thermodynamics of amide + ketone mixtures. 1. Volumetric, speed of sound and refractive index data for N,N-dimethylformamide + 2-alkanone systems at several temperatures
rhoI	801.99	kg/m3	298.15	Thermodynamics of amide + ketone mixtures. 1. Volumetric, speed of sound and refractive index data for N,N-dimethylformamide + 2-alkanone systems at several temperatures

rhoI	806.83	kg/m3	293.15	Thermodynamics of amide + ketone mixtures. 1. Volumetric, speed of sound and refractive index data for N,N-dimethylformamide + 2-alkanone systems at several temperatures
rhoI	796.58	kg/m3	303.15	Excess molar volumes and ultrasonic studies of dimethylsulphoxide with ketones at T = 303.15 K
rhoI	801.52	kg/m3	298.15	Thermodynamics of ketone + amine mixtures. Part X. Excess molarenthalpies at 298.15 K for N,N,N-triethylamine + 2-alkanone systems.Characterization of tertiary amine + 2-alkanone, and of amino-ketone + n-alkane mixtures in terms of DISQUAC
rhoI	801.41	kg/m3	298.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhoI	806.00	kg/m3	293.00	KDB
rhoI	772.43	kg/m3	328.15	Density, Speed of Sound, and Refractive Index Measurements for Binary Mixtures of Pentan-2-one with Propan-2-ol and Butan-2-ol
sfust	54.14	J/mol×K	196.30	NIST Webbook
sfust	2.18	J/mol×K	110.00	NIST Webbook
sfust	54.10	J/mol×K	196.35	NIST Webbook

speedsl	1176.00	m/s	308.15	Densities and Speeds of Sound for Binary Liquid Mixtures of Thiolane-I,I-dioxide with Butanone, Pentan-2-one, Pentan-3-one, and 4-Methyl-pentan-2-one at T = (303.15 or 308.15 or 313.15) K
speedsl	1192.00	m/s	303.15	Densities and Speeds of Sound for Binary Liquid Mixtures of Thiolane-I,I-dioxide with Butanone, Pentan-2-one, Pentan-3-one, and 4-Methyl-pentan-2-one at T = (303.15 or 308.15 or 313.15) K
speedsl	1212.00	m/s	298.15	Vapor liquid equilibria for systems of diethyl carbonate and ketones and determination of group interaction parameters for the UNIFAC and ASOG methods
speedsl	1151.00	m/s	313.15	Densities and Speeds of Sound for Binary Liquid Mixtures of Thiolane-I,I-dioxide with Butanone, Pentan-2-one, Pentan-3-one, and 4-Methyl-pentan-2-one at T = (303.15 or 308.15 or 313.15) K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49654e+01

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.05592e+02
Coeff. B	-8.16731e+03
Coeff. C	-1.36252e+01
Coeff. D	1.10014e-05
Temperature range (K), min.	275.00
Temperature range (K), max.	410.00

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
308.15	101.30	0.0003940
Reference		https://www.doi.org/10.1021/je8003723

Measurement and thermodynamic modeling of ternary (liquid + liquid) phase diagrams of binary mixtures of n-methyl-2-pyrrolidone and ketone. Experimental 2-column chromatographic and gas-liquid equilibria data with thermodynamic properties of Mixtures Containing Ionic Liquids: Activity Coefficients at Infinite Dilution of Organic Compounds in Dilutions of Binary Liquids. Activity coefficients of organic liquids. A methanol-ethanol and ethanol-diisobutylalcohol two liquid systems. Properties of the Binary Ionic Liquid Systems: 1-Allyl-3-methylimidazolium Bromide, 1-Ethyl-3-methylimidazolium Bromide, Cyclohexane, and Carbon Dioxide with Acetone, Ethanolone, Tetrahydrofuran, Composed of Diethyl carbonate, Propylene carbonate and diol at 303.15 K. Interactions between Various Solvents between T = (278.2–323.2) K:

<https://www.doi.org/10.1016/j.jct.2016.09.034>

<https://www.doi.org/10.1016/j.jct.2004.11.007>

<https://www.doi.org/10.1016/j.jct.2007.08.006>

<https://www.doi.org/10.1021/je060033f>

<https://www.doi.org/10.1016/j.jct.2014.04.024>

<https://www.doi.org/10.1021/je500050p>

<https://www.doi.org/10.1021/je050110r>

<https://www.doi.org/10.1021/je025651k>

<https://www.doi.org/10.1021/acs.jced.9b00710>

[illegible]

http://www.elsevier.com/locate/jmb

Exercises: Gas Chromatography:
ethylbenzene/styrene based on limiting activity coefficients:

[illegible][illegible]

Thermodynamics and selectivity of separation based on activity
 Thermodynamics of Ketone + Amine Mixtures. Part V. Molar Excess Activity Coefficients at Infinite Dilution + Density Measurements of Alkanone + Alkanol Mixtures in the Liquid and Supercritical Regions
 Ketone + Alkanol Mixtures for Refractive Index Determination
 Partition Coefficients of Ketones in Ethyl Acetate + Organic Solvents
 Measurements of activity coefficients at infinite dilution of organic systems with ionic liquids: Measurement of γ_{∞} and $\gamma_{\infty}^{\text{H}}$ of 12 organic solutes in ionic liquids using the dynamic method
 Thermodynamic Properties of Some Organic Compounds at Infinite Dilution in Water
 Partition Coefficients at Infinite Dilution and Physicochemical Properties for Organic Solutes in Water and Ionic Liquids
 Thermodynamic Properties for Some Organic Solutes in the Ionic Liquid 1-(3-hydroxypropyl)pyridinium bis(trifluoromethylsulfonyl)amide
 Thermodynamic and Activity Coefficients at Infinite Dilution for Organic Solutes in an Ionic Liquid
 Coefficients at Infinite Dilution for Organic Solutes and Water in the Ionic Liquid 1-butyl-1-methylmorpholinium tricyanomethanide:

<https://www.doi.org/10.1016/j.jct.2016.06.028>
<https://www.doi.org/10.1021/je200333p>
<https://www.doi.org/10.1016/j.jct.2011.02.012>
<https://www.doi.org/10.1021/acs.jced.8b00547>
<https://www.doi.org/10.1016/j.fluid.2015.09.003>
<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
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<https://www.doi.org/10.1016/j.jct.2005.04.010>
<https://www.doi.org/10.1021/je300974g>
<https://www.doi.org/10.1021/acs.jced.7b00035>
<https://www.doi.org/10.1016/j.jct.2013.01.007>
<https://www.doi.org/10.1016/j.jct.2018.01.003>
<https://www.doi.org/10.1016/j.jct.2009.01.006>
<https://www.doi.org/10.1016/j.jct.2011.04.018>
http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
<https://www.doi.org/10.1016/j.jct.2015.02.023>
<https://www.doi.org/10.1016/j.fluid.2018.06.013>
<https://www.doi.org/10.1016/j.jct.2013.08.030>

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhof:	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
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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