

3-Pentanone

Other names:	(C2H5)2CO
	1,3-Dimethylacetone
	DEK
	Diethyl ketone
	Diethylcetone
	Dimethylacetone
	Ethyl ketone
	Ethyl propionyl
	Metacetone
	Methacetone
	NSC 8653
	PROPIONE
	Pentan-3-one
	Pentanone-3
	UN 1156
Inchi:	InChI=1S/C5H10O/c1-3-5(6)4-2/h3-4H2,1-2H3
InchiKey:	FDPIMTJIUBPUKL-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CCC(=O)CC
Mol. weight [g/mol]:	86.13
CAS:	96-22-0

Physical Properties

Property code	Value	Unit	Source
af	0.3440		KDB
affp	836.80	kJ/mol	NIST Webbook
basg	802.60	kJ/mol	NIST Webbook
basg	803.80 ± 0.30	kJ/mol	NIST Webbook
basg	807.00	kJ/mol	NIST Webbook
chl	-3100.20 ± 1.00	kJ/mol	NIST Webbook
chl	-3104.70 ± 0.90	kJ/mol	NIST Webbook
dm	2.70	debye	KDB
gf	-135.40	kJ/mol	KDB
hf	-258.80	kJ/mol	KDB
hf	-253.40 ± 0.90	kJ/mol	NIST Webbook
hf	-257.95 ± 0.84	kJ/mol	NIST Webbook
hf	-260.50 ± 1.60	kJ/mol	NIST Webbook

hfl	-296.51 ± 0.83	kJ/mol	NIST Webbook
hfus	10.30	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
hvap	38.60	kJ/mol	NIST Webbook
hvap	38.52	kJ/mol	NIST Webbook
hvap	38.68	kJ/mol	NIST Webbook
hvap	38.70 ± 0.30	kJ/mol	NIST Webbook
ie	9.32 ± 0.01	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.31 ± 0.02	eV	NIST Webbook
ie	9.37 ± 0.03	eV	NIST Webbook
ie	9.31 ± 0.02	eV	NIST Webbook
ie	9.31	eV	NIST Webbook
ie	9.31 ± 0.01	eV	NIST Webbook
ie	9.22 ± 0.02	eV	NIST Webbook
ie	9.31 ± 0.01	eV	NIST Webbook
log10ws	-0.28		Estimated Solubility Method
log10ws	-0.28		Aqueous Solubility Prediction Method
logp	1.375		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3729.00	kPa	KDB
pc	3729.00 ± 10.00	kPa	NIST Webbook
pc	3740.00 ± 41.40	kPa	NIST Webbook
rhoc	255.81 ± 30.15	kg/m3	NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	705.00		NIST Webbook
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rinpol	701.00	NIST Webbook
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ripol	970.00	NIST Webbook
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ripol	979.00	NIST Webbook
ripol	956.00	NIST Webbook
ripol	970.00	NIST Webbook
ripol	978.00	NIST Webbook
ripol	983.00	NIST Webbook
ripol	983.00	NIST Webbook
ripol	983.00	NIST Webbook
ripol	958.00	NIST Webbook
ripol	976.00	NIST Webbook
ripol	1006.30	NIST Webbook
ripol	1001.50	NIST Webbook
ripol	996.90	NIST Webbook

ripol	1011.30		NIST Webbook
ripol	974.00		NIST Webbook
ripol	977.00		NIST Webbook
sl	266.00	J/molxK	NIST Webbook
tb	375.11	K	KDB
tc	561.46	K	KDB
tc	561.46 ± 0.20	K	NIST Webbook
tc	560.90 ± 0.56	K	NIST Webbook
tc	561.50	K	NIST Webbook
tf	231.20 ± 1.50	K	NIST Webbook
tf	233.35 ± 0.40	K	NIST Webbook
tf	234.18 ± 0.01	K	NIST Webbook
tf	234.15 ± 0.02	K	NIST Webbook
tf	233.90	K	Aqueous Solubility Prediction Method
tf	231.15 ± 0.50	K	NIST Webbook
tf	234.00	K	KDB
tt	234.36	K	Thermodynamics of binary mixtures of N-methyl-2-pyrrolidinone and ketone. Experimental results and modelling of the solid-liquid equilibrium and vapou-liquid equilibrium. The Modified UNIFAC (Do) model characterization
tt	234.16 ± 0.03	K	NIST Webbook
tt	234.16 ± 0.03	K	NIST Webbook
vc	0.336	m3/kmol	KDB
zc	0.2683960		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.14	J/molxK	473.15	NIST Webbook
cpg	168.70	J/molxK	448.15	NIST Webbook
cpg	151.38	J/molxK	383.15	NIST Webbook
cpg	156.77	J/molxK	403.15	NIST Webbook
cpg	162.13	J/molxK	423.15	NIST Webbook
cpg	146.31	J/molxK	364.15	NIST Webbook
cpl	190.00	J/molxK	298.15	NIST Webbook
cpl	190.90	J/molxK	298.15	NIST Webbook
cpl	195.70	J/molxK	298.15	NIST Webbook
cpl	196.40	J/molxK	298.15	NIST Webbook

cpl	190.30	J/molxK	298.15	NIST Webbook
cpl	200.70	J/molxK	298.15	NIST Webbook
dvisc	0.0004190	Paxs	303.15	Density and Viscosity of Binary Mixtures of n-Butyl Acetate with Ketones at (298.15, 303.15, 308.15, and 313.15) K
dvisc	0.0003880	Paxs	313.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Diethyl Oxalate with Some Ketones at (303.15, 308.15, and 313.15) K
dvisc	0.0004490	Paxs	298.15	Density and Viscosity of Binary Mixtures of n-Butyl Acetate with Ketones at (298.15, 303.15, 308.15, and 313.15) K
dvisc	0.0004290	Paxs	303.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Diethyl Oxalate with Some Ketones at (303.15, 308.15, and 313.15) K
dvisc	0.0003960	Paxs	308.15	Density and Viscosity of Binary Mixtures of n-Butyl Acetate with Ketones at (298.15, 303.15, 308.15, and 313.15) K
dvisc	0.0003760	Paxs	313.15	Density and Viscosity of Binary Mixtures of n-Butyl Acetate with Ketones at (298.15, 303.15, 308.15, and 313.15) K

dvisc	0.0003799	Paxs	313.15	Viscosities, Densities, and Ultrasonic Velocities of 3-Pentanone + Ethylbenzene and 3-Pentanone + o-Xylene at (293.15, 303.15, and 313.15) K
dvisc	0.0004231	Paxs	303.15	Viscosities, Densities, and Ultrasonic Velocities of 3-Pentanone + Ethylbenzene and 3-Pentanone + o-Xylene at (293.15, 303.15, and 313.15) K
dvisc	0.0004714	Paxs	293.15	Viscosities, Densities, and Ultrasonic Velocities of 3-Pentanone + Ethylbenzene and 3-Pentanone + o-Xylene at (293.15, 303.15, and 313.15) K
dvisc	0.0003970	Paxs	308.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Diethyl Oxalate with Some Ketones at (303.15, 308.15, and 313.15) K
hfust	11.59	kJ/mol	234.20	NIST Webbook
hfust	0.01	kJ/mol	180.00	NIST Webbook
hfust	0.11	kJ/mol	118.50	NIST Webbook
hfust	11.59	kJ/mol	234.20	NIST Webbook
hvapt	36.90	kJ/mol	303.00	NIST Webbook
hvapt	33.50 ± 0.10	kJ/mol	375.00	NIST Webbook
hvapt	34.90 ± 0.10	kJ/mol	354.00	NIST Webbook
hvapt	36.10 ± 0.10	kJ/mol	335.00	NIST Webbook
hvapt	36.60	kJ/mol	356.50	NIST Webbook
hvapt	33.30	kJ/mol	527.50	NIST Webbook
hvapt	36.60	kJ/mol	377.50	NIST Webbook
hvapt	35.90 ± 0.20	kJ/mol	332.50	NIST Webbook
hvapt	33.45	kJ/mol	375.20	NIST Webbook
hvapt	33.70	kJ/mol	461.50	NIST Webbook

rfi	1.39000		298.15	Phase Equilibria in the Binary and Ternary Systems Composed of Diethyl ketone, 2-Pentanone and 3-Pentanol at 101.3 kPa
rfi	1.39020		298.15	Excess molar volumes and ultrasonic studies of N-methyl-2-pyrrolidone with ketones at T = 303.15 K
rhoI	809.09	kg/m3	298.15	Excess molar enthalpies and volumes of binary mixtures of nonafluorobutylmethylether with ketones at T = 298.15 K
rhoI	818.90	kg/m3	288.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhoI	789.63	kg/m3	318.15	Excess molar volumes, viscosity deviations and excess thermal expansion coefficients for binary and ternary mixtures consist of diethylketone + 2-butanol + ethylchloroacetate at (298.15, 308.15 and 318.15) K
rhoI	814.00	kg/m3	293.00	KDB
rhoI	799.55	kg/m3	308.15	Excess molar volumes, viscosity deviations and excess thermal expansion coefficients for binary and ternary mixtures consist of diethylketone + 2-butanol + ethylchloroacetate at (298.15, 308.15 and 318.15) K

rhoI	809.38	kg/m3	298.15	Excess molar volumes, viscosity deviations and excess thermal expansion coefficients for binary and ternary mixtures consist of diethylketone + 2-butanol + ethylchloroacetate at (298.15, 308.15 and 318.15) K
rhoI	789.41	kg/m3	318.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhoI	804.62	kg/m3	303.15	Excess molar volumes and ultrasonic studies of dimethylsulphoxide with ketones at T = 303.15 K
rhoI	799.32	kg/m3	308.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhoI	809.16	kg/m3	298.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
sfust	0.96	J/molxK	118.50	NIST Webbook
sfust	0.04	J/molxK	180.00	NIST Webbook
sfust	49.50	J/molxK	234.20	NIST Webbook
speedsl	1197.00	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	1179.00	m/s	308.15	Densities and Speeds of Sound for Binary Liquid Mixtures of Thiolane-1,1-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	1160.00	m/s	313.15	Densities and Speeds of Sound for Binary Liquid Mixtures of Thiolane-1,1-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
srf	0.02	N/m	321.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	317.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	307.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	305.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K

srf	0.02	N/m	303.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	311.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	301.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	329.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.03	N/m	297.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.03	N/m	295.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.03	N/m	293.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K

srf	0.03	N/m	291.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	327.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.03	N/m	299.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.03	N/m	289.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	325.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	323.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	319.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K

srf	0.02	N/m	309.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.03	N/m	285.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.03	N/m	283.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	315.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.02	N/m	313.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
srf	0.03	N/m	287.15	Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K

Correlations

Information	Value
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<https://www.doi.org/10.1021/je201129v>

<https://www.doi.org/10.1021/je200195q>

<https://www.doi.org/10.1016/j.jct.2012.01.019>

<https://www.doi.org/10.1021/je300085z>

<https://www.doi.org/10.1016/j.jct.2012.03.005>

<https://www.doi.org/10.1016/j.jct.2016.09.036>

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<https://www.doi.org/10.1016/j.ijct.2015.05.022>

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<https://www.doi.org/10.1016/j.fluid.2018.06.013>

<https://www.doi.org/10.1016/j.ijct.2015.05.014>

<https://www.doi.org/10.1021/ie900056u>

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<https://www.doi.org/10.1016/j.ijet.2014.13.037>

<http://link.springer.com/article/10.1007/BF03311732>

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<https://www.doi.org/10.1016/j.fluid.2007.06.001>

<https://www.doi.org/10.1016/j.fluid.2014.06.031>

<https://www.doi.org/10.1031/acs.joc.2b00326>

<https://www.doi.org/10.1016/j.iast.2023.08.006>

<https://www.doi.org/10.1016/j.jst.2016.06.003>

<http://www.ehri.org/research/ldh/bonarr/bonarr.php?ampid=4496>

<https://www.doi.org/10.1016/j.jst.2019.01.002>

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<http://www.ncbi.nlm.nih.gov/pmc/articles/PMC110101/>

<https://www.industry.gov.au/publications/2018-07-01-10-1010-11-1010-07-017>

<https://www.fishbase.org/portal/portal.jspx?cid=101011>

<https://www.industry.gov.au/publications/industry-2020-2021-annual-report>

<https://www.elsevier.com/locate/jmb>

High selective water/butan-1-ol separation on investigation of limiting separation of water/butan-1-ol based on activity coefficients at infinite dilution and Volumetric Properties of Organic and Aqueous Mixtures at Infinite Dilution

Activity coefficients at infinite dilution of organic solvents and water in 1-ethyl-3-methylimidazolium hexafluorophosphate and 1-butyl-3-methylimidazolium hexafluorophosphate as ionic liquids

Activity coefficients at infinite dilution of organic solutes and water in the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate

Activity coefficients at infinite dilution of organic solutes and water in the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate

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Activity coefficients at infinite dilution of organic solutes and water in the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate

Activity coefficients at infinite dilution of organic solutes and water in the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate

Legend

<https://www.doi.org/10.1016/j.fluid.2017.06.001>

<https://www.doi.org/10.1016/j.jct.2017.10.003>

<https://www.doi.org/10.1021/acs.jced.7b00035>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<https://www.doi.org/10.1016/j.fluid.2016.02.004>

<https://www.doi.org/10.1021/je9003178>

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<https://www.doi.org/10.1021/je700591h>

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af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
srf:	Surface Tension
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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