2-Hexanone

Other names:	2-Oxohexane
	Butyl methyl ketone
	Hexan-2-one
	Hexanone-2
	Ketone, butyl methyl
	MBK
	MNBK
	Methyl butyl ketone
	Methyl n-butyl ketone
	Propylacetone
	n-Butyl methyl ketone
	n-C4H9COCH3
Inchi:	InChI=1S/C6H12O/c1-3-4-5-6(2)7/h3-5H2,1-2H3
InchiKey:	QQZOPKMRPOGIEB-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCCCC(C)=O
Mol. weight [g/mol]:	100.16
CAS:	591-78-6

Physical Properties

Property code	Value	Unit	Source
af	0.3920		KDB
chl	-3754.02 ± 0.96	kJ/mol	NIST Webbook
gf	-129.28	kJ/mol	Joback Method
hf	-279.80 ± 1.10	kJ/mol	NIST Webbook
hfl	-322.00 ± 1.00	kJ/mol	NIST Webbook
hfus	12.89	kJ/mol	Joback Method
hvap	42.22 ± 0.08	kJ/mol	NIST Webbook
hvap	42.20 ± 0.10	kJ/mol	NIST Webbook
hvap	42.90	kJ/mol	NIST Webbook
hvap	43.00 ± 0.30	kJ/mol	NIST Webbook
hvap	43.10 ± 0.10	kJ/mol	NIST Webbook
hvap	43.03	kJ/mol	NIST Webbook
hvap	43.10 ± 0.10	kJ/mol	NIST Webbook
hvap	43.15	kJ/mol	NIST Webbook
ie	9.35 ± 0.06	eV	NIST Webbook
ie	9.44 ± 0.03	eV	NIST Webbook

ie	9.38	eV	NIST Webbook
ie	9.37 ± 0.02	eV	NIST Webbook
ie	9.36 ± 0.02	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.33 ± 0.01	eV	NIST Webbook
ie	9.24 ± 0.02	eV	NIST Webbook
ie	9.34 ± 0.03	eV	NIST Webbook
log10ws	-0.80		Estimated Solubility Method
log10ws	-0.80		Aqueous Solubility Prediction Method
logp	1.766		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	3320.00 ± 80.00	kPa	NIST Webbook
pc	3320.00	kPa	KDB
rhoc	267.42 ± 3.00	kg/m3	NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	768.00		NIST Webbook
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rinpol	792.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	770.00	NIST Webbook
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rinpol	767.90	NIST Webbook
rinpol	767.07	NIST Webbook
rinpol	766.66	NIST Webbook
rinpol	765.86	NIST Webbook
rinpol	766.82	NIST Webbook
rinpol	767.68	NIST Webbook
rinpol	768.37	NIST Webbook
rinpol	768.70	NIST Webbook
rinpol	769.32	NIST Webbook
rinpol	769.68	NIST Webbook
rinpol	771.05	NIST Webbook
rinpol	772.24	NIST Webbook
rinpol	774.21	NIST Webbook
rinpol	788.05	NIST Webbook
rinpol	787.01	NIST Webbook
rinpol	787.84	NIST Webbook
rinpol	789.11	NIST Webbook
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rinpol	767.30	NIST Webbook
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rinpol	728.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	778.00	NIST Webbook
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rinpol	792.00	NIST Webbook
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rinpol	755.00	NIST Webbook
rinpol	792.00	NIST Webbook
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ripol	1098.02	NIST Webbook

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ripol	1077.00		NIST Webbook
ripol	1074.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1107.60		NIST Webbook
sl	308.10	J/mol×K	NIST Webbook
tb	422.90 ± 10.00	K	NIST Webbook
tb	397.15 ± 3.00	K	NIST Webbook
tb	400.30 ± 0.50	K	NIST Webbook
tb	400.70	K	NIST Webbook
tb	401.20	K	NIST Webbook
tb	400.69	K	Isobaric Vapor-Liquid Equilibria of the Ternary System Methylbutyl Ketone + Nonane + Cyclohexanol
tb	400.15 ± 3.00	K	NIST Webbook
tb	400.15 ± 1.00	K	NIST Webbook
tb	400.52 ± 0.50	K	NIST Webbook
tb	400.15 ± 1.00	K	NIST Webbook
tb	400.15 ± 1.00	K	NIST Webbook
tb	399.40 ± 1.00	K	NIST Webbook
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tb	400.70 ± 0.50	K	NIST Webbook
tb	400.15 ± 2.00	K	NIST Webbook
tb	397.65 ± 5.00	K	NIST Webbook
tb	401.15 ± 5.00	K	NIST Webbook
tb	402.15 ± 2.00	K	NIST Webbook
tb	399.15 ± 2.00	K	NIST Webbook
tb	399.65 ± 1.50	K	NIST Webbook
tb	400.95 ± 1.00	K	NIST Webbook
tb	400.35 ± 0.50	K	NIST Webbook
tb	400.75 ± 0.50	K	NIST Webbook
tb	399.00 ± 4.00	K	NIST Webbook

tb	400.70	K	KDB
tb	401.15 ± 1.00	K	NIST Webbook
tb	400.95 ± 0.50	K	NIST Webbook
tc	587.00	K	KDB
tc	586.60 ± 0.40	K	NIST Webbook
tc	587.00	K	NIST Webbook
tc	587.00 ± 0.50	K	NIST Webbook
tf	216.25 ± 0.30	K	NIST Webbook
tf	217.60	K	KDB
tf	217.03	K	Aqueous Solubility Prediction Method
tt	218.42	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	217.69 ± 0.05	K	NIST Webbook
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.63	J/mol×K	568.08	Joback Method
cpg	187.80	J/mol×K	420.14	Joback Method
cpg	197.51	J/mol×K	449.73	Joback Method
cpg	206.83	J/mol×K	479.31	Joback Method
cpg	215.79	J/mol×K	508.90	Joback Method
cpg	224.39	J/mol×K	538.49	Joback Method
cpg	177.72	J/mol×K	390.55	Joback Method
cpl	213.30	J/mol×K	298.15	NIST Webbook
cpl	213.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0003010	Pa×s	390.55	Joback Method
dvisc	0.0011124	Pa×s	268.39	Joback Method
dvisc	0.0019023	Pa×s	237.85	Joback Method
dvisc	0.0038104	Pa×s	207.31	Joback Method
dvisc	0.0005126	Pa×s	329.47	Joback Method
dvisc	0.0003840	Pa×s	360.01	Joback Method
dvisc	0.0007258	Pa×s	298.93	Joback Method
hfust	14.90	kJ/mol	217.69	NIST Webbook

hfust	14.90	kJ/mol	217.70	NIST Webbook
hfust	14.90	kJ/mol	217.70	NIST Webbook
hvapt	39.00	kJ/mol	380.00	NIST Webbook
hvapt	40.80	kJ/mol	352.00	NIST Webbook
hvapt	43.80	kJ/mol	351.00	NIST Webbook
hvapt	42.50 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	36.70	kJ/mol	472.00	NIST Webbook
hvapt	36.10	kJ/mol	550.00	NIST Webbook
hvapt	53.80	kJ/mol	340.00	NIST Webbook
hvapt	39.50 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	40.10 ± 0.10	kJ/mol	348.00	NIST Webbook
hvapt	40.70 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	43.10	kJ/mol	400.70	NIST Webbook
hvapt	41.60 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	36.35	kJ/mol	400.70	NIST Webbook
hvapt	41.50	kJ/mol	368.50	NIST Webbook
rfi	1.40080		293.13	Isobaric Vapor-Liquid Equilibria of the Ternary System Methylbutyl Ketone + 1-Pentanol + Anisole
rfi	1.40080		293.15	Isobaric Vapor-Liquid Equilibria of the Ternary System Methylbutyl Ketone + 1-Pentanol + Nonane
rhol	797.60	kg/m3	308.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhol	788.45	kg/m3	318.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhol	806.70	kg/m3	298.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water

rhol	815.72	kg/m3	288.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhol	806.37	kg/m3	298.20	Liquid-liquid equilibrium for methyl butyl ketone + o-, m-, p-cresol + water ternary systems and COSMO-SAC predictions
rhol	816.00	kg/m3	288.00	KDB
rhol	811.00	kg/m3	293.20	Ternary and Quaternary Liquid-Liquid Equilibria for Systems of Methyl Butyl Ketone + Water + Hydroquinone + Phenol at 313.2 K and Atmospheric Pressure
sfust	68.44	J/mol×K	217.69	NIST Webbook
sfust	68.42	J/mol×K	217.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38679e+01
Coeff. B	-2.82795e+03
Coeff. C	-9.42620e+01
Temperature range (K), min.	302.50
Temperature range (K), max.	424.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.75253e+00
Coeff. B	-5.04800e+03
Coeff. C	2.29627e+00

Coeff. D	-8.15597e-06
Temperature range (K), min.	217.35
Temperature range (K), max.	587.05

Sources

Activity Coefficients at Infinite Dilution of Organic Solutes and Water in Tributylethylphosphonium Diethylphosphate Using Gas Liquid Chromatography: Thermodynamic Properties of Mixtures Containing Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.5b00980
(Liquid + liquid) phase equilibria of 1-alkyl-3-methylimidazolium methylsulfate with alcohols, or ethers, or ketones:	https://www.doi.org/10.1016/j.jct.2005.07.024
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Activity coefficients at infinite dilution measurements for organic solutes and water in the ionic liquid 1-ethyl-3-methylimidazolium tetracyanoborate:	https://www.doi.org/10.1016/j.jct.2011.02.012
Ternary and Quaternary Liquid-Liquid Equilibria for Systems of Methyl Butyl Ketone + Water + Hydroquinone + Phenol at 313.2 K and Atmospheric Pressure:	https://www.doi.org/10.1021/acs.jced.5b00918
Liquid-liquid equilibrium for methyl butyl ketone + o, m, p-cresol + water ternary systems and COSMO-SAC predictions:	https://www.doi.org/10.1016/j.jct.2018.07.014
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Experimental and theoretical study on infinite dilution activity coefficients of various solutes in piperidinium ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.01.005
Henry s Constants of 1-Alkanols and 2-Ketones in Salt Solutions:	https://www.doi.org/10.1021/je0600956
Thermodynamics of binary mixtures of N-methyl-2-pyrrolidinone and ketone. Experimental results and modelling of the solid-liquid equilibrium and vapour-liquid equilibrium. The Modified UNIFAC (Do) model characterization:	https://www.doi.org/10.1016/j.jct.2004.11.007
Measurements of activity coefficients at infinite dilution for organic solutes and water in N-hexylisoquinolinium thiocyanate, [HiQuin][SCN] using GLC:	https://www.doi.org/10.1016/j.jct.2013.02.004
Solubility measurement, model evaluation and thermodynamic analysis of rivaroxaban polymorphs in organic solvents:	https://www.doi.org/10.1016/j.jct.2016.09.036
Activity coefficients at infinite dilution for organic solutes and water in 1-ethyl-1-methylpyrrolidinium lactate:	https://www.doi.org/10.1016/j.jct.2015.05.014
The study of activity coefficients at infinite dilution for organic solutes and water in 1-butyl-4-methylpyridinium dicyanamide, [B4MPy][DCA] using GLC:	https://www.doi.org/10.1016/j.jct.2013.09.007
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1198
Liquid Liquid Equilibria for Ternary Systems: Methyl Butyl Ketone + Phenol + Water and Methyl Butyl Ketone + Hydroquinone + Water at 298.15 K and 323.15 K:	https://www.doi.org/10.1021/je500532v
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591786&Units=SI
Air-Water Partitioning of C5 and C6 Alkanones: Measurement, Critical Compilation, Correlation, and Recommended Data:	https://www.doi.org/10.1021/acs.jced.9b00726
Phase Equilibria of (1-Ethyl-3-methylimidazolium Ethylsulfate + Hydrocarbon, + Ketone, and + Ether) Binary Systems:	https://www.doi.org/10.1021/je700591h
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
A relative headspace method for Henry s constants of volatile organic compounds:	https://www.doi.org/10.1016/j.fluid.2005.02.006
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1198
A thermodynamic study of the ketoreductase-catalyzed reduction of 2-alkanones in non-aqueous solvents:	https://www.doi.org/10.1016/j.jct.2004.08.002
Measurements of activity coefficients at infinite dilution of organic solutes and water in 1-propyl-1-methylpiperidinium bis{(trifluoromethyl)sulfonyl}imide ionic liquid using g.l.c.:	https://www.doi.org/10.1016/j.jct.2010.05.017
Isobaric Vapor-Liquid Equilibria of the Ternary System Methylbutyl Ketone + [illegible]	https://www.doi.org/10.1021/je900058p
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Legend

af:	Acentric Factor
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
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
rhol:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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