2-Butanone, 3-methyl-

Other names:	2-Acetylpropane
	2-Methylbutan-3-one
	3-METHYL-2-BUTANONE
	3-Methyl-2-butanoate
	3-Methylbutan-2-one
	3-methylbutanone
	Isopropyl methyl ketone
	Ketone, isopropyl methyl
	METHYLBUTANONE
	MIPK
	Methyl butanone-2
	Methyl isopropyl ketone
	NSC 9379
	UN 2397
	iso-C3H7COCH3
Inchi:	InChI=1S/C5H10O/c1-4(2)5(3)6/h4H,1-3H3
InchiKey:	SYBYTAAJFKOIEJ-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CC(=O)C(C)C
Mol. weight [g/mol]:	86.13
CAS:	563-80-4

Physical Properties

Property code	Value	Unit	Source
af	0.3310		KDB
affp	836.30	kJ/mol	NIST Webbook
basg	804.40	kJ/mol	NIST Webbook
chl	-3097.20 ± 0.80	kJ/mol	NIST Webbook
dm	2.80	debye	KDB
gf	-140.14	kJ/mol	Joback Method
hf	-262.57 ± 0.87	kJ/mol	NIST Webbook
hfl	-299.47 ± 0.86	kJ/mol	NIST Webbook
hfus	6.78	kJ/mol	Joback Method
hvap	36.90	kJ/mol	NIST Webbook
hvap	36.80	kJ/mol	NIST Webbook
hvap	36.87	kJ/mol	NIST Webbook
hvap	36.81	kJ/mol	NIST Webbook

ie	9.31 ± 0.02	eV	NIST Webbook
ie	9.30 ± 0.04	eV	NIST Webbook
ie	9.36	eV	NIST Webbook
ie	9.30 ± 0.01	eV	NIST Webbook
ie	9.30 ± 0.02	eV	NIST Webbook
ie	9.30 ± 0.01	eV	NIST Webbook
ie	9.30 ± 0.01	eV	NIST Webbook
ie	9.32 ± 0.02	eV	NIST Webbook
log10ws	-0.12		Aqueous Solubility Prediction Method
log10ws	-0.12		Estimated Solubility Method
logp	1.231		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	3850.00	kPa	KDB
pc	3800.00 ± 20.00	kPa	NIST Webbook
pc	3850.00 ± 48.30	kPa	NIST Webbook
rhoc	278.21 ± 24.98	kg/m3	NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	640.90		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	640.90		NIST Webbook
rinpol	642.78		NIST Webbook
rinpol	639.36		NIST Webbook
rinpol	639.89		NIST Webbook
rinpol	640.49		NIST Webbook
rinpol	641.53		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	642.00		NIST Webbook

rinpol	646.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	650.00	NIST Webbook
rinpol	647.20	NIST Webbook
rinpol	636.00	NIST Webbook
rinpol	673.00	NIST Webbook
rinpol	640.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	641.00	NIST Webbook
rinpol	641.00	NIST Webbook
rinpol	666.10	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	638.00	NIST Webbook
rinpol	659.00	NIST Webbook
rinpol	654.00	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	639.00	NIST Webbook
rinpol	637.00	NIST Webbook
rinpol	658.00	NIST Webbook
rinpol	641.00	NIST Webbook
rinpol	653.00	NIST Webbook
rinpol	640.00	NIST Webbook
rinpol	640.00	NIST Webbook
rinpol	641.00	NIST Webbook
rinpol	642.00	NIST Webbook
rinpol	641.53	NIST Webbook
ripol	965.00	NIST Webbook
ripol	954.40	NIST Webbook
ripol	959.60	NIST Webbook
ripol	943.20	NIST Webbook
ripol	929.00	NIST Webbook
ripol	936.00	NIST Webbook
ripol	929.00	NIST Webbook
ripol	929.00	NIST Webbook
ripol	918.00	NIST Webbook
ripol	929.00	NIST Webbook
ripol	927.00	NIST Webbook
ripol	989.00	NIST Webbook
ripol	956.00	NIST Webbook
ripol	929.00	NIST Webbook
ripol	929.00	NIST Webbook
ripol	970.00	NIST Webbook
ripol	949.00	NIST Webbook
ripol	936.00	NIST Webbook

ripol	918.00		NIST Webbook
ripol	929.00		NIST Webbook
ripol	965.00		NIST Webbook
ripol	949.40		NIST Webbook
ripol	925.00		NIST Webbook
sl	268.50	J/mol×K	NIST Webbook
tb	367.65 ± 2.00	K	NIST Webbook
tb	366.65 ± 1.00	K	NIST Webbook
tb	366.65 ± 1.00	K	NIST Webbook
tb	366.65 ± 1.00	K	NIST Webbook
tb	367.65 ± 2.00	K	NIST Webbook
tb	365.55 ± 0.30	K	NIST Webbook
tb	366.65 ± 1.00	K	NIST Webbook
tb	366.15 ± 1.00	K	NIST Webbook
tb	367.65 ± 2.00	K	NIST Webbook
tb	367.15 ± 1.00	K	NIST Webbook
tb	368.30 ± 2.00	K	NIST Webbook
tb	367.48	K	KDB
tb	368.65 ± 1.00	K	NIST Webbook
tb	366.65 ± 1.00	K	NIST Webbook
tb	366.70 ± 0.50	K	NIST Webbook
tb	365.15 ± 2.00	K	NIST Webbook
tb	368.15 ± 2.00	K	NIST Webbook
tb	366.65 ± 1.00	K	NIST Webbook
tb	366.65 ± 1.00	K	NIST Webbook
tb	365.65 ± 5.00	K	NIST Webbook
tb	366.65 ± 2.00	K	NIST Webbook
tb	366.15 ± 1.00	K	NIST Webbook
tb	367.30 ± 1.00	K	NIST Webbook
tb	365.15 ± 5.00	K	NIST Webbook
tb	367.41 ± 0.50	K	NIST Webbook
tb	368.15 ± 2.00	K	NIST Webbook
tb	366.65 ± 1.00	K	NIST Webbook
tb	365.65 ± 2.00	K	NIST Webbook
tb	368.55 ± 2.00	K	NIST Webbook
tb	367.35 ± 0.50	K	NIST Webbook
tb	366.15 ± 2.00	K	NIST Webbook
tb	367.90 ± 0.50	K	NIST Webbook
tb	367.65 ± 1.00	K	NIST Webbook
tb	367.35 ± 0.50	K	NIST Webbook
tb	367.70	K	NIST Webbook
tb	367.40	K	NIST Webbook
tb	389.50 ± 0.30	K	NIST Webbook
tb	367.65 ± 1.00	K	NIST Webbook

tb	367.15 ± 1.00	K	NIST Webbook
tb	368.60 ± 0.50	K	NIST Webbook
tb	368.30 ± 0.60	K	NIST Webbook
tb	368.00 ± 0.40	K	NIST Webbook
tc	553.40 ± 0.83	K	NIST Webbook
tc	553.40	K	NIST Webbook
tc	553.10 ± 0.40	K	NIST Webbook
tc	553.40	K	KDB
tf	181.00	K	KDB
tf	178.75 ± 0.40	K	NIST Webbook
tf	181.15 ± 0.60	K	NIST Webbook
tf	180.78	K	Aqueous Solubility Prediction Method
tt	180.01 ± 0.06	K	NIST Webbook
vc	0.310	m3/kmol	KDB
zc	0.2593860		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.09	J/mol×K	473.15	NIST Webbook
cpg	166.77	J/mol×K	453.15	NIST Webbook
cpg	161.25	J/mol×K	433.15	NIST Webbook
cpg	154.26	J/mol×K	408.15	NIST Webbook
cpg	146.82	J/mol×K	383.15	NIST Webbook
cpg	139.58	J/mol×K	358.15	NIST Webbook
cpl	179.90	J/mol×K	298.15	NIST Webbook
cpl	180.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0005129	Pa×s	305.17	Joback Method
dvisc	0.0012505	Pa×s	243.10	Joback Method
dvisc	0.0002843	Pa×s	367.23	Joback Method
dvisc	0.0023744	Pa×s	212.07	Joback Method
dvisc	0.0056166	Pa×s	181.04	Joback Method
dvisc	0.0003716	Pa×s	336.20	Joback Method
dvisc	0.0007615	Pa×s	274.13	Joback Method
hfust	9.34	kJ/mol	180.00	NIST Webbook
hfust	9.34	kJ/mol	180.00	NIST Webbook
hfust	9.34	kJ/mol	180.01	NIST Webbook
hvapt	35.50	kJ/mol	340.00	NIST Webbook
hvapt	32.30 ± 0.10	kJ/mol	367.00	NIST Webbook
hvapt	32.35	kJ/mol	367.40	NIST Webbook

hvapt	32.60	kJ/mol	452.50	NIST Webbook
hvapt	33.80	kJ/mol	389.00	NIST Webbook
hvapt	35.00 ± 0.10	kJ/mol	327.00	NIST Webbook
hvapt	35.00	kJ/mol	352.50	NIST Webbook
hvapt	33.80 ± 0.10	kJ/mol	346.00	NIST Webbook
rfi	1.38620		298.15	Vapor-Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Methylpentane, 3-Methyl-2-butanone and 3-Methyl-2-butanol
rfi	1.38620		298.15	Isothermal vapour liquid equilibria in the binary and ternary systems composed of 2-propanol, 3-methyl-2-butanone and 2,2,4-trimethylpentane
rhol	798.51	kg/m3	298.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhol	803.00	kg/m3	293.00	KDB
rhol	808.30	kg/m3	288.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhol	800.63	kg/m3	298.15	Liquid-liquid equilibria for the pseudo-ternary system {aqueous sulfuric acid solution + methyl ethyl ketone or methyl isopropyl ketone + phosphonium-based ionic liquids} at 298.15 K and atmospheric pressure

rhol	799.55	kg/m3	298.15	Vapour-liquid equilibria in binary and ternary systems composed of 2,3-dimethylbutane, diisopropyl ether, and 3-methyl-2-butanone at 313.15, 323.15 and 313.15 K
rhol	788.60	kg/m3	308.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
rhol	778.62	kg/m3	318.15	Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water
sfust	51.90	J/mol×K	180.01	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42556e+01
Coeff. B	-2.91500e+03
Coeff. C	-6.45290e+01
Temperature range (K), min.	273.22
Temperature range (K), max.	390.44

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.01851e+02
Coeff. B	-1.16914e+04
Coeff. C	-2.86327e+01
Coeff. D	2.74487e-05
Temperature range (K), min.	181.15
Temperature range (K), max.	553.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1195.mol
Vapor-Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Methylpentane, 3-Methyl-2-butanone and 3-Methyl-2-butanol:	https://www.doi.org/10.1021/je050062a
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1195
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Ternary liquid-liquid equilibria for methyl isopropyl ketone + (resorcinol or hydroquinone) + water systems at different temperatures:	https://www.doi.org/10.1016/j.fluid.2016.08.040
Screening solvents to extract phenol from aqueous solutions by the COSMO-SAC model and extraction process simulation:	https://www.doi.org/10.1016/j.fluid.2017.08.007
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1195
Isothermal vapour liquid equilibria in the binary and ternary systems composed of 2-propanol, 3-methyl-2-butanone and 2,2,4-trimethylpentane:	https://www.doi.org/10.1016/j.fluid.2007.10.016
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Experimental result and data correlation of liquid-liquid equilibrium for methyl isopropyl ketone + o,m,p-dihydroxybenzene + water at 333.15 K, 343.15 K and 353.15 K:	https://www.doi.org/10.1016/j.jct.2018.08.041
Vapour-liquid equilibria in binary and ternary systems composed of 2,3-dimethylbutane, diisopropyl ether, and 3-methyl-2-butanone at 313.15, 323.15 and 333.15 K:	https://www.doi.org/10.1016/j.fluid.2013.01.020
Air-Water Partitioning of C5 and C6 Alkanones: Measurement, Critical Compilation, Correlation, and Recommended Data:	https://www.doi.org/10.1021/acs.jced.9b00726
Activity coefficients at infinite dilution for different alcohols and ketones in [EMpy][ESO4]: Experimental data and modeling with PC-SAFT:	https://www.doi.org/10.1016/j.fluid.2015.09.003
Experimental Determination and Correlation of Liquid-Liquid Equilibria for Methyl Isopropyl Ketone + Phenol + Water Mixtures at 298.15, 313.15, and 323.15 K:	https://www.doi.org/10.1021/acs.jced.5b00895
Thermal and Volumetric Properties of Some C5 and C6 Alkanones at Infinite Dilution in Water:	https://www.doi.org/10.1021/acs.jced.7b00035
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C563804&Units=SI
Determination and modeling of liquid-liquid equilibrium for ternary mixtures of methyl isopropyl ketone, cresol isomers and water:	https://www.doi.org/10.1016/j.fluid.2016.08.034
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Extraction of o-, m- and p-cresol from aqueous solution with methyl isopropyl ketone: Equilibrium, correlations, and COSMO-RS predictions:	https://www.doi.org/10.1016/j.jct.2017.07.033
Salting-out effect of NaCl and KCl on the ternary LLE data for the systems of (water + propionic acid + isopropyl methyl ketone) and of (water + propionic acid + isobutyl methyl ketone):	https://www.doi.org/10.1016/j.jct.2003.11.011
Liquid-liquid equilibria for the pseudoternary system {aqueous sulfuric acid solution + methyl ethyl ketone or methyl isopropyl ketone + phosphonium-based ionic liquids} at 298.15 K and atmospheric pressure:	https://www.doi.org/10.1016/j.fluid.2013.07.054

Legend

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
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
zc:	Critical Compressibility