Acetylacetone

Other names:	2,4-Dioxopentane
	2,4-PENTANEDIONE
	2,4-Pentadione
	2,4-Pentandione
	2-Propanone, acetyl-
	ACAC
	ACETOACETONE
	Acetone, acetyl-
	Acetyl 2-propanone
	CH3COCH2COCH3
	DIACETYLMETHANE
	NSC 5575
	Pentan-2,4-dione
	Pentane-2,4-dione
	Pentanedione
	Pentanedione-2,4
	UN 2310
Inchi:	InChI=1S/C5H8O2/c1-4(6)3-5(2)7/h3H2,1-2H3
InchiKey:	YRKCREAYFQTBPV-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC(=O)CC(C)=O
Mol. weight [g/mol]:	100.12
CAS:	123-54-6

Physical Properties

Property code	Value	Unit	Source
affp	873.50	kJ/mol	NIST Webbook
basg	836.80	kJ/mol	NIST Webbook
chl	-2581.90	kJ/mol	NIST Webbook
chl	-2687.00 ± 1.50	kJ/mol	NIST Webbook
chl	-2667.00 ± 12.00	kJ/mol	NIST Webbook
chl	-2685.40 ± 0.80	kJ/mol	NIST Webbook
gf	-266.62	kJ/mol	Joback Method
hf	-376.10 ± 2.00	kJ/mol	NIST Webbook
hf	-420.10	kJ/mol	NIST Webbook
hf	-384.40 ± 1.30	kJ/mol	NIST Webbook
hfl	-427.60 ± 1.10	kJ/mol	NIST Webbook

hfl	-528.94	kJ/mol	NIST Webbook
hfl	-414.10 ± 2.00	kJ/mol	NIST Webbook
hfl	-447.30 ± 8.00	kJ/mol	NIST Webbook
hfus	11.90	kJ/mol	Joback Method
hvap	43.20 ± 1.00	kJ/mol	NIST Webbook
hvap	41.78	kJ/mol	NIST Webbook
hvap	43.20 ± 0.10	kJ/mol	NIST Webbook
ie	9.63 ± 0.01	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.18 ± 0.07	eV	NIST Webbook
ie	8.85 ± 0.02	eV	NIST Webbook
ie	8.85 ± 0.05	eV	NIST Webbook
ie	8.82 ± 0.02	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	8.87 ± 0.03	eV	NIST Webbook
log10ws	0.22		Aqueous Solubility Prediction Method
logp	0.554		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	4046.64	kPa	Joback Method
rinpol	760.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	786.60		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	786.60		NIST Webbook
rinpol	787.25		NIST Webbook
rinpol	763.43		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	799.00		NIST Webbook

rinpol	754.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	804.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1196.00		NIST Webbook
tb	413.60	K	NIST Webbook
tb	409.15 ± 2.00	K	NIST Webbook
tb	410.70 ± 2.00	K	NIST Webbook
tb	413.60	K	Isobaric Vapor-Liquid Equilibria for (Acetic Acid + Cyclohexane) and (Cyclohexane + Acetylacetone) at a Pressure of 101.3 kPa and for (Acetic Acid + Acetylacetone) at a Pressure of 60.0 kPa
tb	410.15 ± 0.40	K	NIST Webbook
tb	411.10	K	NIST Webbook
tb	410.15 ± 1.50	K	NIST Webbook
tb	411.00	K	NIST Webbook
tb	409.15 ± 2.00	K	NIST Webbook
tb	410.65 ± 1.50	K	NIST Webbook
tc	613.03	K	Joback Method
tf	249.95 ± 0.30	K	NIST Webbook
tt	254.80 ± 0.20	K	NIST Webbook
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.02	J/mol×K	613.03	Joback Method
cpg	164.27	J/mol×K	453.45	Joback Method
cpg	172.09	J/mol×K	485.37	Joback Method
cpg	179.57	J/mol×K	517.28	Joback Method
cpg	186.71	J/mol×K	549.20	Joback Method
cpg	193.52	J/mol×K	581.11	Joback Method
cpg	156.11	J/mol×K	421.54	Joback Method
dvisc	0.0006090	Pa×s	308.15	Viscosity Behavior of Some Oxygen Containing Compounds
dvisc	0.0006700	Pa×s	298.15	Viscosity Behavior of Some Oxygen Containing Compounds
dvisc	0.0007410	Pa×s	288.15	Viscosity Behavior of Some Oxygen Containing Compounds
hvapt	39.40	kJ/mol	347.50	NIST Webbook
hvapt	35.20	kJ/mol	394.50	NIST Webbook
hvapt	42.70	kJ/mol	333.00	NIST Webbook
hvapt	34.30	kJ/mol	411.10	NIST Webbook
hvapt	39.20	kJ/mol	360.50	NIST Webbook
hvapt	40.60	kJ/mol	304.00	NIST Webbook
rfi	1.45110		293.15	(Vapor + liquid) equilibrium of the binary mixtures formed by acetonitrile with selected compounds at 95.5 kPa
rfi	1.44890		293.15	Liquid-Liquid Equilibrium of (Water + Pentane-2,4-dione + Ethyl Ethanoate) and (Water + Pentane-2,4-dione + Cyclohexane) at (298.15 and 313.15) K

rfi	1.45090		298.15	Liquid-Liquid Equilibrium, Solid-Liquid Equilibrium, Densities, and Refractivity of a Water, Chloroform, and Acetylacetone Mixture
rfi	1.44910		298.15	Isobaric Vapor Liquid Equilibria for Binary Systems of Acetone + Isopropenyl Acetate, 2-Butanone + Isopropenyl Acetate, and Isopropenyl Acetate + Acetylacetone at 101.3 kPa
rfi	1.44910		293.15	Isobaric Vapor-Liquid Equilibria for the Binary Systems of Acetic Acid + Isopropenyl Acetate, Acetic Acid + Acetylacetone, and Water + Acetylacetone
rhol	939.30	kg/m3	328.15	Determination and correlation of molar excess enthalpies of binary systems 2,4-pentanedione + (1-butanol, + 2-methyl-1-propanol, + 1-pentanol, + 1-heptane, + ethyl acetate, and + water)
rhol	954.00	kg/m3	313.15	Determination and correlation of molar excess enthalpies of binary systems 2,4-pentanedione + (1-butanol, + 2-methyl-1-propanol, + 1-pentanol, + 1-heptane, + ethyl acetate, and + water)

rhol	972.10	kg/m3	298.15	Determination and correlation of molar excess enthalpies of binary systems 2,4-pentanedione + (1-butanol, + 2-methyl-1-propanol, + 1-pentanol, + 1-heptane, + ethyl acetate, and + water)	
rhol	971.07	kg/m3	298.15	Liquid-liquid equilibria, excess molar volume and deviations of the refractive indices at 298.15 K for mixtures of solvents used in themolybdenum extraction process	
rhol	972.00	kg/m3	298.15	Bubble point measurements of binary mixtures formed by ethyl benzene with selected compounds at 95.35 kPa	
rhol	972.10	kg/m3	298.15	Excess Enthalpies of 2,4-Pentanedione + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (298.15, 313.15, and 328.15) K and p = (0.1 and 10.0) MPa	
rhol	954.00	kg/m3	313.15	Excess Enthalpies of 2,4-Pentanedione + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (298.15, 313.15, and 328.15) K and p = (0.1 and 10.0) MPa	

rhol	939.30	kg/m3	328.15	Excess Enthalpies of 2,4-Pentanedione + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (298.15, 313.15, and 328.15) K and p = (0.1 and 10.0) MPa
srf	0.03	N/m	298.15	Concentration Dependence of Surface Tension for Very Dilute Aqueous Solutions of Organic Non-Electrolytes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.20	K	99.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37695e+01
Coeff. B	-3.02532e+03
Coeff. C	-8.04060e+01
Temperature range (K), min.	304.80
Temperature range (K), max.	438.09

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.91943e+02
Coeff. B	-1.67244e+04
Coeff. C	-4.19801e+01

Coeff. D	3.58083e-05
Temperature range (K), min.	249.95
Temperature range (K), max.	602.00

Sources

Solubility of 1,1'-(Butane-1,4-diyl)-bis(3-methylpyridinium) Dihexafluorophosphate in Different Solvents from (288.15 to 338.15) K:	https://www.doi.org/10.1021/je9010954
Concentration Dependence of Surface Tension for Very Dilute Aqueous Solutions of Organic Non-Electrolytes	https://www.doi.org/10.1021/je049955d
Solubility of Organic Compounds in Ternary systems of water + acetyl acetone + propyl acetate at several temperatures:	https://www.doi.org/10.1016/j.fluid.2010.11.029
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1193
Excess Enthalpies of 2,4-Pentanedione + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (298.15, 313.15, and 328.15) K and p = (0.1 and 10) MPa:	https://www.doi.org/10.1021/je700492k
Liquid-liquid equilibria, excess molar volume and deviations of the refractive properties at 298.15 K for mixtures of 1,1'-(Butane-1,4-diyl)-bis(3-methyl-1H-imidazolium-1-yl) Dihexafluorophosphate + (Water + Acetone + Cyclohexane):	https://www.doi.org/10.1016/j.fluid.2013.06.013
Solubility and Solvent Effect Study of Ethyl Ethanoate Extraction Process:	https://www.doi.org/10.1021/je900826p
Liquid-Liquid Equilibrium of Water + Acetone + Cyclohexane + Ethyl Ethanoate) at (298.15 and 313.15) K:	https://www.doi.org/10.1021/je100704j
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Isobaric Vapor-Liquid Equilibria for (Acetic Acid + Cyclohexane) and (Cyclohexane + Acetylacetone) at a Pressure of 101.3 kPa:	https://www.doi.org/10.1021/je900669t
Isobaric Vapor-Liquid Equilibria for the Binary Systems of Acetic Acid + Acetylacetone, and Water + Acetylacetone:	https://www.doi.org/10.1021/je800345j
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid-Liquid Equilibrium, Solid-Liquid Equilibrium, Densities, and Refractivity of a Water + Chloroform and Acetylacetone Mixture:	https://www.doi.org/10.1021/je100747y
Bubble point measurements of binary mixtures formed by ethyl benzene with Solubility of Compounds at 95.35 kPa:	https://www.doi.org/10.1016/j.jct.2008.05.002
1,1'-(Ethane-1,2-diyl)-bis(3-methylpyridinium) Dihexafluorophosphate in Different Solvents:	https://www.doi.org/10.1021/je900627q
Viscosity Behavior of Some Oxygen Containing Compounds:	https://www.doi.org/10.1007/s10765-010-0860-3
Isobaric Vapor Liquid Equilibria for Binary Systems of Acetone + Isopropenyl Acetate, 2-Butanone + Isopropenyl Acetate, and Isopropenyl Acetate + Acetylacetone at 101.3 kPa:	https://www.doi.org/10.1021/je700605t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Measurement of Infinite Dilution Activity Coefficients of Alcohols, Ketones, and Aromatic Hydrocarbons in Ionic Liquids Using Gas–Liquid Chromatography:	https://www.doi.org/10.1021/je800246v
(Vapor + liquid) equilibrium of the binary mixtures formed by acetonitrile + methanol or ethanol and 1-Butyl-3-methylimidazolium Hexafluorophosphate at 95.5 kPa:	https://www.doi.org/10.1016/j.jct.2007.03.007
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Determination and correlation of molar excess enthalpies of binary systems containing 2,4-pentanedione + (1-butanol, + 2-methyl-2-propanol, + 1-pentanol, + 1-heptanol, + ethyl acetate, and + 1,12-(Propane-1,3-diyl)-bis(3-methyl-1H-imidazolium-1-yl) Dihexafluorophosphate in Different Solvents:	https://www.doi.org/10.1016/j.fluid.2007.12.008
KDB Vapor Pressure Data:	https://www.doi.org/10.1021/je9006585
	https://www.cheric.org/files/research/kdb/mol/mol1193.mol
	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1193
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123546&Units=SI
Critical Assessment of CO2 Solubility in Volatile Solvents at 298.15 K:	https://www.doi.org/10.1021/je101161d

Legend

affp:	Proton affinity

basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume