Cyclopentanone

Other names:	ADIPIC KETONE
	Adipinketon
	DUMASIN
	KETOCYCLOPENTANE
	Ketopentamethylene
	NSC 4122
	UN 2245
Inchi:	InChI=1S/C5H8O/c6-5-3-1-2-4-5/h1-4H2
InchiKey:	BGTOWKSIORTVQH-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	O=C1CCCC1
Mol. weight [g/mol]:	84.12
CAS:	120-92-3

Physical Properties

Property code	Value	Unit	Source
af	0.3500		KDB
affp	828.00 ± 4.00	kJ/mol	NIST Webbook
affp	823.70	kJ/mol	NIST Webbook
basg	794.00	kJ/mol	NIST Webbook
chl	-2874.00 ± 0.92	kJ/mol	NIST Webbook
chl	-2870.00 ± 0.80	kJ/mol	NIST Webbook
chl	-2873.50 ± 1.60	kJ/mol	NIST Webbook
dm	3.00	debye	KDB
ea	0.00	eV	NIST Webbook
gf	-87.11	kJ/mol	Joback Method
hf	-197.40 ± 1.30	kJ/mol	NIST Webbook
hf	-194.80 ± 1.70	kJ/mol	NIST Webbook
hf	-192.80	kJ/mol	KDB
hf	-193.00 ± 1.80	kJ/mol	NIST Webbook
hfl	-240.20 ± 1.30	kJ/mol	NIST Webbook
hfl	-236.50	kJ/mol	NIST Webbook
hfl	-237.40 ± 1.70	kJ/mol	NIST Webbook
hfus	1.08	kJ/mol	Joback Method
hvap	42.60 ± 0.40	kJ/mol	NIST Webbook
hvap	42.77	kJ/mol	NIST Webbook
hvap	42.72	kJ/mol	NIST Webbook

hvap	42.70 ± 0.10	kJ/mol	NIST Webbook
hvap	42.63 ± 0.42	kJ/mol	NIST Webbook
hvap	42.10 ± 0.20	kJ/mol	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	9.42 ± 0.03	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	9.25 ± 0.02	eV	NIST Webbook
ie	9.28 ± 0.01	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	9.26 ± 0.01	eV	NIST Webbook
ie	9.25 ± 0.02	eV	NIST Webbook
ie	9.26 ± 0.01	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-1.09		Crippen Method
logp	1.129		Crippen Method
mcvol	72.020	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4600.00	kPa	KDB
pc	4600.00 ± 50.00	kPa	NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	116.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	741.10		NIST Webbook
rinpol	740.90		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	749.60		NIST Webbook
rinpol	793.80		NIST Webbook

rinpol	766.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	116.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	802.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	761.10	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	767.00	NIST Webbook
ripol	1187.00	NIST Webbook
ripol	1168.00	NIST Webbook
ripol	1154.00	NIST Webbook
ripol	1166.00	NIST Webbook
ripol	1211.70	NIST Webbook
ripol	1176.00	NIST Webbook
ripol	1176.00	NIST Webbook
ripol	1185.00	NIST Webbook
ripol	1168.00	NIST Webbook
ripol	1168.00	NIST Webbook
ripol	1167.00	NIST Webbook
ripol	1200.00	NIST Webbook
ripol	1144.00	NIST Webbook

ripol	1150.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1211.70		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1203.10		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1206.30		NIST Webbook
ripol	1166.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1172.00		NIST Webbook
ripol	1154.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1202.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1176.00		NIST Webbook
ripol	1154.00		NIST Webbook
ripol	1186.00		NIST Webbook
ripol	1170.00		NIST Webbook
tb	403.72	K	KDB
tc	624.50 ± 2.00	K	NIST Webbook
tc	624.50	K	KDB
tf	221.85 ± 0.50	K	NIST Webbook
tf	221.85 ± 0.40	K	NIST Webbook
tf	221.80	K	KDB
tf	222.60 ± 0.60	K	NIST Webbook
tf	220.05 ± 0.50	K	NIST Webbook
tf	221.70 ± 0.30	K	NIST Webbook
tt	221.44 ± 0.02	K	NIST Webbook
tt	220.77	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
vc	0.268	m3/kmol	KDB
zc	0.2374230		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.04	J/mol×K	460.00	NIST Webbook
cpg	139.31	J/mol×K	440.00	NIST Webbook
cpg	133.86	J/mol×K	420.00	NIST Webbook
cpg	128.03	J/mol×K	400.00	NIST Webbook
cpg	121.16	J/mol×K	375.00	NIST Webbook
cpg	149.22	J/mol×K	480.00	NIST Webbook
cpg	116.90	J/mol×K	360.00	NIST Webbook
dvisc	0.0008610	Pa×s	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	0.0010840	Pa×s	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	0.0008650	Pa×s	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	0.0009270	Pa×s	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
dvisc	0.0009990	Pa×s	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	0.0009230	Pa×s	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	0.0009980	Pa×s	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
hfust	11.40	kJ/mol	221.20	NIST Webbook
hfust	11.40	kJ/mol	221.20	NIST Webbook
hvapt	41.50	kJ/mol	363.00	NIST Webbook
hvapt	40.60	kJ/mol	372.00	NIST Webbook
hvapt	42.60	kJ/mol	348.50	NIST Webbook
hvapt	36.35	kJ/mol	403.70	NIST Webbook
hvapt	43.60	kJ/mol	286.00	NIST Webbook
hvapt	39.60	kJ/mol	377.00	NIST Webbook
rfi	1.43470		298.15	Vapour pressure and excess Gibbs energy of binary 1,2-dichloroethane + cyclohexanone, chloroform + cyclopentanone and chloroform + cyclohexanone mixtures at temperatures from 298.15 to 318.15 K
rfi	1.43470		298.15	Isothermal (vapour + liquid) equilibria in the binary mixtures (1,2-dichloroethane and 1,1,1-trichloroethane with cyclopentanone) within the temperature range (298.15 to 313.15) K

rfi	1.43490		298.15	Isothermal (vapour + liquid) equilibria for the binary (cyclopentanone or cyclohexanone with 1,1,2,2-tetrachloroethane) systems at temperatures of (343.15, 353.15, and 363.15) K
rfi	1.43470		298.15	Isothermal (vapour + liquid) equilibria and excess Gibbs free energies in some binary (cyclopentanone + chloroalkane) mixtures at temperatures from 298.15 K to 318.15 K
rhol	950.00	kg/m3	293.00	KDB
rhol	924.99	kg/m3	318.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K
rhol	934.69	kg/m3	308.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K
rhol	944.35	kg/m3	298.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K

rhol	953.99	kg/m3	288.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K	
rhol	944.30	kg/m3	298.15	Excess molar enthalpies for binary mixtures of cyclopentanone, cyclohexanone, or cycloheptanone with n-nonane at T = 298.15 K and atmospheric pressure	
rhol	945.00	kg/m3	298.15	Phase equilibrium relations for binary mixed hydrate systemscomposed of carbon dioxide and cyclopentane derivatives	
rhol	949.90	kg/m3	293.15	Phase equilibrium relations for binary mixed hydrate systemscomposed of carbon dioxide and cyclopentane derivatives	
rhol	954.70	kg/m3	288.15	Phase equilibrium relations for binary mixed hydrate systemscomposed of carbon dioxide and cyclopentane derivatives	
rhol	959.50	kg/m3	283.15	Phase equilibrium relations for binary mixed hydrate systemscomposed of carbon dioxide and cyclopentane derivatives	

rhol	964.30	kg/m3	278.15	Phase equilibrium relations for binary mixed hydrate systemscomposed of carbon dioxide and cyclopentane derivatives
rhol	969.10	kg/m3	273.15	Phase equilibrium relations for binary mixed hydrate systemscomposed of carbon dioxide and cyclopentane derivatives
srf	0.03	N/m	298.15	Concentration Dependence of Surface Tension for Very Dilute Aqueous Solutions of Organic Non-Electrolytes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54060e+01
Coeff. B	-3.97854e+03
Coeff. C	-3.49970e+01
Temperature range (K), min.	298.15
Temperature range (K), max.	429.12

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.04761e+02
Coeff. B	-8.53493e+03
Coeff. C	-1.34566e+01
Coeff. D	1.06922e-05
Temperature range (K), min.	221.85
Temperature range (K), max.	626.00

Sources

Solubility Determination, Modeling, and Thermodynamic Dissolution Properties of Benzenesulfonamide in 16 Neat Solvents from 273.15 to 324.45 K:	https://www.doi.org/10.1021/acs.jced.9b00360
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic Parameters of a New Synthesized Tricationic Ionic Liquid Stationary Phase by Inverse Gas Chromatography:	https://www.doi.org/10.1021/acs.jced.8b00601
Solubility Measurement and Thermodynamic Modeling for o-Toluenesulfonamide in 16 Solvents from T = 273.15 to 323.85 K:	https://www.doi.org/10.1021/acs.jced.9b00445
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess molar enthalpies for binary mixtures of cyclopentanone, cyclohexanone, or cycloheptanone with n-nonane at T = 298.15 K and atmospheric pressure:	https://www.doi.org/10.1016/j.jct.2014.03.007
Odd Even Effects in the Static Dielectric Permittivity of a Homologous Series of Liquid Cycloalkanones, (CH2)n-1C-O, n = 4 to 8:	https://www.doi.org/10.1021/je200682t
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120923&Units=SI
Vapour pressure and excess Gibbs energy of binary 1,2-dichloroethane + cyclohexanone, chloroform + cyclopentanone and chloroform + cyclohexanone mixtures at temperatures from 298.15 to 318.15 K:	https://www.doi.org/10.1016/j.fluid.2008.02.018
Excess molar volumes and excess isentropic compressibilities of ternary [illegible]ds and [illegible]	https://www.doi.org/10.1016/j.jct.2017.04.013
Density and Viscosity of Binary Mixtures of n-Butyl Acetate with Ketones at (298.15, 303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je300085z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isothermal (vapour + liquid) equilibria and excess Gibbs free energies in some binary (cyclopentanone + chloroalkane) mixtures at temperatures from 298.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2007.03.008
Thermodynamic properties of ternary mixtures containing 1-ethyl-3-methylimidazolium tetrafluoroborate with cyclic amides and cyclopentanone or cyclohexanone at T = (293.15, 298.15, 303.15 and 308.15) K:	https://www.doi.org/10.1016/j.jct.2015.02.018
(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
Phase equilibrium relations for binary mixed hydrate systems composed of carbon dioxide and cyclopentane derivatives:	https://www.doi.org/10.1016/j.fluid.2013.10.057
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
Partial molar volumes of organic solutes in water. XXIII. Cyclic ketones at (298 to 573) K and pressures to 30 MPa:	https://www.doi.org/10.1016/j.jct.2011.02.010
Concentration Dependence of Surface Tension for Very Dilute Aqueous Solutions of Organic Non-Electrolytes:	https://www.doi.org/10.1021/je049955d
Solvation parameter model and thermodynamic parameters in a dicationic ionic liquid based on pyrrolidinium:	https://www.doi.org/10.1016/j.jct.2014.12.023
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1223
Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je901052w
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1223.mol
Liquid-Liquid Extraction of Cyclopentanone from Aqueous Solution with Methylcyclohexane or Propyl Acetate at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.7b01109
Measurement of activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-hexyl-1,4-diaza[2.2.2]bicyclooctanium bis(trifluoromethylsulfonyl)imide using gas-liquid chromatography:	https://www.doi.org/10.1016/j.jct.2013.10.026
Isothermal (vapour + liquid) equilibria in the binary mixtures (1,2-dibromoethane and [illegible] + cyclopentanone) within the temperature range (298.15 to 313.15) K:	https://www.doi.org/10.1016/j.jct.2005.07.016
Densities, Viscosities, and Refractive Indices of Binary Mixtures of Diethyl Carbonate with Some Ketones at (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je100715x
Isothermal (vapour + liquid) equilibria for the binary (cyclopentanone or cyclohexanone with 1,1,2,2-tetrachloroethane) systems at temperatures of (343.15, 353.15, and 363.15) K:	https://www.doi.org/10.1016/j.jct.2006.01.010
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermophysical Properties and Solubility of Different Sugar-Derived Molecules in Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.7b00184
Henry's Law Constants of Organic Compounds in Water and n-Octane at T = 293.2 K:	https://www.doi.org/10.1021/je900711h

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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