1-Propanone, 1-phenyl-

Other names:	1-Phenyl-1-propanone
	1-phenylpropanone
	Ethyl phenyl ketone
	Ketone, ethyl phenyl
	NSC 16937
	Phenyl ethyl ketone
	Propionylbenzene
	Propiophenone
	USAF EK-1235
Inchi:	InChI=1S/C9H10O/c1-2-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3
InchiKey:	KRIOVPPHQSLHCZ-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CCC(=O)c1ccccc1
Mol. weight [g/mol]:	134.18
CAS:	93-55-0

Physical Properties

Property code	Value	Unit	Source
affp	867.40	kJ/mol	NIST Webbook
basg	835.60	kJ/mol	NIST Webbook
chl	-4803.70 ± 1.00	kJ/mol	NIST Webbook
ea	0.35 ± 0.00	eV	NIST Webbook
gf	8.39	kJ/mol	Joback Method
hf	-105.14	kJ/mol	Joback Method
hfl	-167.20 ± 1.30	kJ/mol	NIST Webbook
hfus	14.71	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
ie	9.27 ± 0.05	eV	NIST Webbook
ie	9.16	eV	NIST Webbook
log10ws	-1.83		Aqueous Solubility Prediction Method
logp	2.279		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1178.00		NIST Webbook

rinpol	1179.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1180.30		NIST Webbook
rinpol	1172.80		NIST Webbook
rinpol	1165.30		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1188.60		NIST Webbook
rinpol	1183.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1696.00		NIST Webbook
tb	490.85 ± 1.00	K	NIST Webbook
tb	490.70	K	NIST Webbook
tb	481.15 ± 10.00	K	NIST Webbook
tb	489.15 ± 2.00	K	NIST Webbook
tb	490.90 ± 0.50	K	NIST Webbook
tb	471.15 ± 10.00	K	NIST Webbook
tc	704.23	K	Joback Method
tf	291.76 ± 0.05	K	NIST Webbook
tf	291.55	K	Aqueous Solubility Prediction Method
tf	288.15 ± 1.50	K	NIST Webbook
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.47	J/mol×K	485.87	Joback Method
cpg	258.54	J/mol×K	558.66	Joback Method
cpg	299.72	J/mol×K	704.23	Joback Method
cpg	269.91	J/mol×K	595.05	Joback Method
cpg	280.54	J/mol×K	631.45	Joback Method
cpg	290.46	J/mol×K	667.84	Joback Method
cpg	246.41	J/mol×K	522.26	Joback Method
dvisc	0.0003454	Pa×s	449.48	Joback Method
dvisc	0.0004578	Pa×s	413.09	Joback Method
dvisc	0.0006407	Pa×s	376.71	Joback Method
dvisc	0.0009636	Pa×s	340.32	Joback Method
dvisc	0.0015978	Pa×s	303.93	Joback Method
dvisc	0.0002719	Pa×s	485.87	Joback Method
dvisc	0.0030402	Pa×s	267.54	Joback Method
hvapt	44.40	kJ/mol	422.50	NIST Webbook
hvapt	52.10	kJ/mol	505.50	NIST Webbook
rfi	1.52450		298.15	Excess Molar Volumes of (propiophenone + benzene, or toluene, or ethylbenzene, or butylbenzene) at temperatures 298.15 K and 328.15 K
rfi	1.52450		298.15	Excess molar volumes of (propiophenone + toluene) and estimated density of liquid propiophenone below its melting temperature
rhol	1009.20	kg/m3	298.15	Ultrasonic Studies of Binary Mixtures of Some Aromatic Ketones with N-Methyl-acetamide at 308.15 K
speedsl	1432.00	m/s	308.15	Ultrasonic studies on binary mixtures of some aromatic ketones with acetonitrile at T = 308.15 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44716e+01
Coeff. B	-4.07036e+03
Coeff. C	-7.75510e+01
Temperature range (K), min.	364.52
Temperature range (K), max.	521.91

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
308.15	101.30	0.0014680

Reference *https://www.doi.org/10.1016/j.jct.2005.05.006*

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	1005.3
298.15	2130.00	1006.4
298.15	4150.00	1007.5
298.15	6180.00	1008.7
298.15	8210.00	1009.8
298.15	10230.00	1010.9
298.15	11250.00	1011.5
298.15	12260.00	1012.1
298.15	14290.00	1013.2

298.15	16310.00	1014.3
298.15	18340.00	1015.3
298.15	20370.00	1016.4
298.15	22390.00	1017.5
298.15	24420.00	1018.5
298.15	26450.00	1019.5
298.15	28470.00	1020.5
298.15	29490.00	1021.0
298.15	30500.00	1021.6
298.15	32530.00	1022.5
298.15	34550.00	1023.5
298.15	36580.00	1024.5
298.15	38600.00	1025.5
298.15	39620.00	1025.9
308.15	100.00	996.8
308.15	2130.00	998.0
308.15	4150.00	999.2
308.15	6180.00	1000.4
308.15	8210.00	1001.6
308.15	10230.00	1002.8
308.15	11250.00	1003.4
308.15	12260.00	1003.9
308.15	14290.00	1005.1
308.15	16310.00	1006.2
308.15	18340.00	1007.3
308.15	20370.00	1008.4
308.15	22390.00	1009.5
308.15	24420.00	1010.6
308.15	26450.00	1011.7
308.15	28470.00	1012.8
308.15	29490.00	1013.2
308.15	30500.00	1013.8
308.15	32530.00	1014.8
308.15	34550.00	1015.8
308.15	36580.00	1016.8
308.15	38600.00	1017.9
308.15	39620.00	1018.3
318.15	100.00	988.3
318.15	2130.00	989.6
318.15	4150.00	990.9
318.15	6180.00	992.1
318.15	8210.00	993.3
318.15	10230.00	994.6
318.15	11250.00	995.2

318.15	12260.00	995.8
318.15	14290.00	997.0
318.15	16310.00	998.1
318.15	18340.00	999.3
318.15	20370.00	1000.4
318.15	22390.00	1001.6
318.15	24420.00	1002.7
318.15	26450.00	1003.8
318.15	28470.00	1004.9
318.15	29490.00	1005.5
318.15	30500.00	1006.0
318.15	32530.00	1007.1
318.15	34550.00	1008.2
318.15	36580.00	1009.2
318.15	38600.00	1010.3
318.15	39620.00	1010.8
328.15	100.00	979.6
328.15	2130.00	981.1
328.15	4150.00	982.4
328.15	6180.00	983.7
328.15	8210.00	985.0
328.15	10230.00	986.2
328.15	11250.00	986.9
328.15	12260.00	987.5
328.15	14290.00	988.7
328.15	16310.00	990.0
328.15	18340.00	991.2
328.15	20370.00	992.3
328.15	22390.00	993.5
328.15	24420.00	994.7
328.15	26450.00	995.9
328.15	28470.00	997.1
328.15	29490.00	997.6
328.15	30500.00	998.2
328.15	32530.00	999.3
328.15	34550.00	1000.4
328.15	36580.00	1001.5
328.15	38600.00	1002.6
328.15	39620.00	1003.2

Reference *https://www.doi.org/10.1016/j.jct.2004.10.011*

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Ultrasonic studies on binary mixtures of some aromatic ketones with acetonitrile at T = 308.15 K:	https://www.doi.org/10.1016/j.jct.2006.01.009
(P, Vm, T) Measurements of (toluene + propiophenone) at temperatures from 298.15 K to 328.15 K and at pressures up to 40 MPa:	https://www.doi.org/10.1016/j.jct.2004.10.011
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C93550&Units=SI
Excess Molar Volumes of (propiophenone + benzene, or toluene, or ethylbenzene, or butylbenzene) at temperatures 298.15 K and 328.15 K:	https://www.doi.org/10.1016/j.jct.2005.01.007
Density and viscosity of binary liquid systems of N-methylacetamide with aromatic ketones at T = 308.15 K:	https://www.doi.org/10.1016/j.jct.2005.05.006
Excess molar volumes of (propiophenone + toluene) and estimated density of liquid propiophenone below its melting temperature:	https://www.doi.org/10.1016/j.jct.2005.12.008
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Ultrasonic Studies of Binary Mixtures of Some Aromatic Ketones with N-Methyl acetamide at 308.15 K:	https://www.doi.org/10.1021/je040008e
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume