4-Heptanone

Other names:	(n-C3H7)2CO
	BUTYRONE
	Di-n-propyl ketone
	Dipropyl ketone
	GBL
	Heptan-4-one
	NSC 8692
	PROPYL KETONE
	UN 2710
Inchi:	InChI=1S/C7H14O/c1-3-5-7(8)6-4-2/h3-6H2,1-2H3
InchiKey:	HCFAJYNVAYBARA-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCCC(=O)CCC
Mol. weight [g/mol]:	114.19
CAS:	123-19-3

Physical Properties

Property code	Value	Unit	Source
affp	845.00	kJ/mol	NIST Webbook
basg	815.30	kJ/mol	NIST Webbook
gf	-120.86	kJ/mol	Joback Method
hf	-298.30 ± 1.30	kJ/mol	NIST Webbook
hfus	15.49	kJ/mol	Joback Method
hvap	47.80	kJ/mol	NIST Webbook
hvap	46.20 ± 0.40	kJ/mol	NIST Webbook
hvap	46.70	kJ/mol	NIST Webbook
ie	9.84	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	9.10 ± 0.01	eV	NIST Webbook
ie	9.12 ± 0.03	eV	NIST Webbook
ie	9.10 ± 0.04	eV	NIST Webbook
ie	9.04 ± 0.02	eV	NIST Webbook
log10ws	-1.30		Estimated Solubility Method
log10ws	-1.30		Aqueous Solubility Prediction Method
logp	2.156		Crippen Method

mcvol	111.060	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	2995.87	kPa	Joback Method
rhoc	262.63 ± 3.43	kg/m3	NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	853.40		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	853.40		NIST Webbook

rinpol	857.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	872.00		NIST Webbook
ripol	1131.90		NIST Webbook
ripol	1131.90		NIST Webbook
ripol	1135.50		NIST Webbook
ripol	1118.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1151.10		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1139.40		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1157.10		NIST Webbook
ripol	1118.00		NIST Webbook
ripol	1157.10		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1120.80		NIST Webbook
tb	418.40 ± 1.00	K	NIST Webbook
tb	419.15 ± 2.00	K	NIST Webbook
tb	417.15 ± 1.00	K	NIST Webbook
tb	416.70 ± 0.50	K	NIST Webbook
tb	417.20 ± 0.50	K	NIST Webbook
tb	417.65 ± 1.00	K	NIST Webbook
tb	416.65 ± 2.00	K	NIST Webbook
tb	417.15 ± 0.50	K	NIST Webbook
tb	416.15 ± 3.00	K	NIST Webbook
tb	415.40 ± 1.50	K	NIST Webbook
tb	424.65 ± 5.00	K	NIST Webbook
tb	416.65 ± 1.00	K	NIST Webbook
tb	414.65 ± 5.00	K	NIST Webbook
tb	415.65 ± 3.00	K	NIST Webbook
tb	417.20	K	NIST Webbook
tb	416.67	K	KDB
tb	416.15 ± 2.00	K	NIST Webbook
tb	419.15 ± 2.00	K	NIST Webbook
tb	416.05 ± 2.00	K	NIST Webbook
tb	415.65 ± 2.00	K	NIST Webbook

tb	417.40 ± 0.50	K	NIST Webbook
tb	417.25 ± 0.50	K	NIST Webbook
tb	417.23 ± 0.20	K	NIST Webbook
tb	417.15 ± 1.00	K	NIST Webbook
tb	418.15 ± 1.00	K	NIST Webbook
tb	416.65 ± 0.50	K	NIST Webbook
tb	416.65 ± 1.00	K	NIST Webbook
tb	413.15 ± 5.00	K	NIST Webbook
tb	413.15 ± 5.00	K	NIST Webbook
tb	416.67 ± 0.20	K	NIST Webbook
tb	416.70 ± 1.00	K	NIST Webbook
tb	414.15 ± 3.00	K	NIST Webbook
tc	602.00 ± 0.20	K	NIST Webbook
tf	240.70 ± 0.50	K	NIST Webbook
tf	240.60 ± 0.20	K	NIST Webbook
tt	241.77	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	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.81	J/mol×K	442.86	Joback Method
cpg	237.73	J/mol×K	472.29	Joback Method
cpg	248.21	J/mol×K	501.71	Joback Method
cpg	258.27	J/mol×K	531.14	Joback Method
cpg	267.92	J/mol×K	560.57	Joback Method
cpg	277.17	J/mol×K	590.00	Joback Method
cpg	215.46	J/mol×K	413.43	Joback Method
dvisc	0.0005212	Pa×s	348.48	Joback Method
dvisc	0.0007459	Pa×s	316.00	Joback Method
dvisc	0.0003871	Pa×s	380.95	Joback Method
dvisc	0.0020181	Pa×s	251.05	Joback Method
dvisc	0.0041439	Pa×s	218.58	Joback Method
dvisc	0.0003013	Pa×s	413.43	Joback Method
dvisc	0.0011589	Pa×s	283.53	Joback Method

hfust	16.16	kJ/mol	240.20	NIST Webbook
hfust	17.53	kJ/mol	236.00	NIST Webbook
hfust	16.16	kJ/mol	240.20	NIST Webbook
hvapt	40.70	kJ/mol	303.00	NIST Webbook
hvapt	57.50	kJ/mol	356.50	NIST Webbook
hvapt	45.50	kJ/mol	397.00	NIST Webbook
pvap	40.00	kPa	385.47	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane
pvap	40.00	kPa	385.50	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane
pvap	91.55	kPa	413.43	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane
pvap	86.20	kPa	411.20	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane
pvap	78.55	kPa	407.98	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane

pvap	69.39	kPa	403.74	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane
pvap	59.15	kPa	398.38	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane
pvap	50.95	kPa	393.78	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane
pvap	43.17	kPa	388.63	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane
pvap	36.63	kPa	383.70	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane

pvap	29.93	kPa	377.77	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane	
pvap	22.69	kPa	370.01	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane	
pvap	17.72	kPa	363.42	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane	
pvap	14.54	kPa	358.74	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane	
pvap	40.00	kPa	385.87	Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane	

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50215e+01
Coeff. B	-3.74392e+03
Coeff. C	-5.71180e+01
Temperature range (K), min.	311.22
Temperature range (K), max.	442.69

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.51465e+02
Coeff. B	-1.08461e+04
Coeff. C	-2.05602e+01
Coeff. D	1.80628e-05
Temperature range (K), min.	267.15
Temperature range (K), max.	405.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123193&Units=SI
Phase Equilibria of (1-Ethyl-3-methylimidazolium Ethylsulfate + Hydrocarbon, + Ketone, and + Ether) Binary Systems:	https://www.doi.org/10.1021/je700591h
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1206
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs Comprising 2-, 3-, and 4-Heptanone with n-Octane, n-Nonane, and n-Decane:	https://www.doi.org/10.1021/je500731x
Thermodynamics of binary mixtures of N-methyl-2-pyrrolidinone and ketone. Experimental results and modelling of liquid–liquid phase equilibria of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide with alcohols, ethers, or ketones:	https://www.doi.org/10.1016/j.jct.2004.11.007
Experimental results and modelling of the solid–liquid equilibrium and liquid–liquid phase equilibria of 1-alkyl-3-methylimidazolium dialkylsulfate with alcohols, ethers, or ketones:	https://www.doi.org/10.1016/j.jct.2005.07.024
Vapour–liquid equilibrium. The Modified Cripen (mc) model characterization:	https://www.cheric.org/files/research/kdb/mol/mol1206.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity

basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume