

3-Heptanone

Other names:	3-Oxoheptane Aethylbutylketon Butyl ethyl ketone ETHYLBUTYLCETONE Eptan-3-one Ethyl butyl ketone Ethyl n-butyl ketone Ethylbutylketon Etilbutilchetone HEPTAN-3-ONE Heptan-3-on NSC 8448 n-Butyl ethyl ketone n-C4H9COC2H5 n-Heptan-3-one
Inchi:	InChI=1S/C7H14O/c1-3-5-6-7(8)4-2/h3-6H2,1-2H3
InchiKey:	NGAZZOYFWWSOGK-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCCCC(=O)CC
Mol. weight [g/mol]:	114.19
CAS:	106-35-4

Physical Properties

Property code	Value	Unit	Source
gf	-120.86	kJ/mol	Joback Method
hf	-300.39	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	37.92	kJ/mol	Joback Method
ie	9.15 ± 0.09	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.02 ± 0.02	eV	NIST Webbook
ie	9.15 ± 0.02	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
log10ws	-2.03		Crippen Method
logp	2.156		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB

nfpah	%!d(float64=1)		KDB
pc	2995.87	kPa	Joback Method
rhoc	263.77 ± 3.43	kg/m3	NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	884.10		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	869.42		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	887.40		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	865.00		NIST Webbook

rinpol	880.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	869.00	NIST Webbook
rinpol	861.00	NIST Webbook
rinpol	869.00	NIST Webbook
rinpol	866.50	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	869.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	866.20	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	865.80	NIST Webbook
rinpol	866.20	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	865.80	NIST Webbook
rinpol	860.00	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	887.50	NIST Webbook
ripol	1160.00	NIST Webbook
ripol	1160.00	NIST Webbook
ripol	1185.00	NIST Webbook
ripol	1167.00	NIST Webbook
ripol	1171.00	NIST Webbook
ripol	1141.00	NIST Webbook
ripol	1124.00	NIST Webbook
ripol	1155.00	NIST Webbook
ripol	1167.00	NIST Webbook
ripol	1162.00	NIST Webbook
ripol	1155.00	NIST Webbook
ripol	1157.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1163.00	NIST Webbook
ripol	1131.00	NIST Webbook
ripol	1185.00	NIST Webbook
ripol	1167.20	NIST Webbook
ripol	1173.20	NIST Webbook

ripol	1179.90		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1161.00		NIST Webbook
tb	420.45	K	NIST Webbook
tb	422.65 ± 5.00	K	NIST Webbook
tb	420.70	K	NIST Webbook
tb	420.65 ± 4.00	K	NIST Webbook
tb	420.20 ± 0.50	K	NIST Webbook
tb	414.15 ± 2.00	K	NIST Webbook
tb	416.65 ± 3.00	K	NIST Webbook
tb	420.15 ± 3.00	K	NIST Webbook
tb	418.90 ± 3.00	K	NIST Webbook
tb	418.65 ± 3.00	K	NIST Webbook
tb	420.55 ± 0.50	K	NIST Webbook
tb	420.75 ± 0.50	K	NIST Webbook
tb	420.95 ± 1.00	K	NIST Webbook
tb	420.80 ± 0.60	K	NIST Webbook
tb	418.65 ± 3.00	K	NIST Webbook
tc	606.60 ± 0.25	K	NIST Webbook
tf	420.45	K	NIST Webbook
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.17	J/mol×K	590.00	Joback Method
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	215.46	J/mol×K	413.43	Joback Method
dvisc	0.0003871	Pa×s	380.95	Joback Method
dvisc	0.0005212	Pa×s	348.48	Joback Method
dvisc	0.0007459	Pa×s	316.00	Joback Method
dvisc	0.0011589	Pa×s	283.53	Joback Method

dvisc	0.0020181	Pa×s	251.05	Joback Method
dvisc	0.0003013	Pa×s	413.43	Joback Method
dvisc	0.0041439	Pa×s	218.58	Joback Method
hfust	17.53	kJ/mol	236.00	NIST Webbook
pvap	32.58	kPa	383.09	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	27.11	kPa	377.99	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	54.02	kPa	398.84	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	64.03	kPa	404.44	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	74.50	kPa	409.63	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	82.00	kPa	412.95	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	90.50	kPa	416.50	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	40.00	kPa	388.11	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	388.36	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	388.67	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	23.27	kPa	373.60	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	18.75	kPa	367.95	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	15.51	kPa	363.03	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	12.93	kPa	358.58	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	11.05	kPa	354.82	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	39.13	kPa	388.62	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	45.12	kPa	393.02	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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50665e+01
Coeff. B	-3.78159e+03
Coeff. C	-5.80630e+01
Temperature range (K), min.	313.94
Temperature range (K), max.	445.72

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	8.40676e+01
Coeff. B	-8.19745e+03
Coeff. C	-1.01131e+01
Coeff. D	6.53118e-06
Temperature range (K), min.	354.15
Temperature range (K), max.	404.15

Sources

KDB:	https://www.chemic.org/files/research/kdb/mol/mol1205.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.chemic.org/research/kdb/hcprop/showprop.php?cmpid=1205
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapor Liquid Equilibria Measurements for the Nine n-Alkane/Ketone Pairs (n-Heptane, n-Octane, n-Nonane, and n-Decane)	https://www.doi.org/10.1021/je500731x
Non-polar Retention Indices and Correlation of liquid-liquid equilibrium data for the ternary mixtures of n-Heptane + water)	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106354&Units=SI
The Yaws Handbook of Vapor Pressure: Experimental Determination and Modeling of Liquid-Liquid Equilibrium for Binary Mixtures of Ethylene Glycol + 1,2-Butanediol + 3-Heptanone or Anisole:	https://www.doi.org/10.1016/j.jct.2016.11.004 https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure https://www.doi.org/10.1021/acs.jced.8b01257 http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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
vc:	Critical Volume

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