3-Hexanone

Other names:	Aethylpropylketon
	Ethyl n-propyl ketone
	Ethyl propyl ketone
	Hexan-3-one
	Hexanone-(3)
	n-C3H7COC2H5
Inchi:	InChI=1S/C6H12O/c1-3-5-6(7)4-2/h3-5H2,1-2H3
InchiKey:	PFCHFHIRKBAQGU-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCCC(=O)CC
Mol. weight [g/mol]:	100.16
CAS:	589-38-8

Physical Properties

Property code	Value	Unit	Source
af	0.3780		KDB
affp	843.20	kJ/mol	NIST Webbook
basg	811.30	kJ/mol	NIST Webbook
chl	-3755.90 ± 0.79	kJ/mol	NIST Webbook
gf	-129.28	kJ/mol	Joback Method
hf	-278.25 ± 0.89	kJ/mol	NIST Webbook
hfl	-320.13 ± 0.86	kJ/mol	NIST Webbook
hfus	12.89	kJ/mol	Joback Method
hvap	35.70	kJ/mol	Joback Method
ie	9.30	eV	NIST Webbook
ie	9.12 ± 0.02	eV	NIST Webbook
log10ws	-0.83		Estimated Solubility Method
log10ws	-0.83		Aqueous Solubility Prediction Method
logp	1.766		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3320.00	kPa	KDB
pc	3320.00 ± 20.00	kPa	NIST Webbook
rhoc	265.42 ± 3.00	kg/m3	NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	781.00		NIST Webbook

rinpol	761.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	787.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	746.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	802.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	746.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	764.80	NIST Webbook
rinpol	765.97	NIST Webbook
rinpol	764.11	NIST Webbook
rinpol	764.10	NIST Webbook
rinpol	764.37	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	750.00	NIST Webbook

rinpol	761.00	NIST Webbook
rinpol	746.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	751.00	NIST Webbook
rinpol	757.40	NIST Webbook
rinpol	783.30	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	785.50	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	795.00	NIST Webbook
ripol	1051.00	NIST Webbook
ripol	1084.50	NIST Webbook
ripol	1068.00	NIST Webbook
ripol	1055.00	NIST Webbook
ripol	1073.30	NIST Webbook
ripol	1048.00	NIST Webbook
ripol	1042.00	NIST Webbook
ripol	1052.00	NIST Webbook
ripol	1055.00	NIST Webbook
ripol	1068.00	NIST Webbook
ripol	1075.00	NIST Webbook
ripol	1072.00	NIST Webbook
ripol	1078.90	NIST Webbook
ripol	1052.00	NIST Webbook
ripol	1055.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1055.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1042.00	NIST Webbook
ripol	1057.00	NIST Webbook
ripol	1053.00	NIST Webbook
ripol	1053.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1053.00	NIST Webbook
ripol	1027.00	NIST Webbook
ripol	1060.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1047.00	NIST Webbook
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ripol	1053.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1053.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1053.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1053.00		NIST Webbook
ripol	1023.00		NIST Webbook
ripol	1049.00		NIST Webbook
ripol	1040.00		NIST Webbook
sg	409.60	J/mol×K	NIST Webbook
sl	305.30	J/mol×K	NIST Webbook
tb	396.60	K	KDB
tc	582.80	K	NIST Webbook
tc	582.82	K	KDB
tc	583.20 ± 0.25	K	NIST Webbook
tc	582.82 ± 0.40	K	NIST Webbook
tf	217.60	K	KDB
tf	217.90	K	Aqueous Solubility Prediction Method
tf	217.50 ± 0.01	K	NIST Webbook
tf	217.48 ± 0.02	K	NIST Webbook
tt	217.72 ± 0.05	K	NIST Webbook
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.92	J/mol×K	423.15	NIST Webbook
cpg	178.45	J/mol×K	383.15	NIST Webbook
cpg	200.41	J/mol×K	448.15	NIST Webbook
cpg	208.03	J/mol×K	473.15	NIST Webbook
cpg	215.81	J/mol×K	498.15	NIST Webbook
cpg	185.14	J/mol×K	403.15	NIST Webbook
cpl	216.90	J/mol×K	298.15	NIST Webbook
cpl	216.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0007258	Pa×s	298.93	Joback Method
dvisc	0.0038104	Pa×s	207.31	Joback Method
dvisc	0.0005126	Pa×s	329.47	Joback Method

dvisc	0.0003840	Pa×s	360.01	Joback Method
dvisc	0.0011124	Pa×s	268.39	Joback Method
dvisc	0.0019023	Pa×s	237.85	Joback Method
dvisc	0.0003010	Pa×s	390.55	Joback Method
hfust	13.47	kJ/mol	217.70	NIST Webbook
hfust	0.68	kJ/mol	145.00	NIST Webbook
hfust	13.47	kJ/mol	217.70	NIST Webbook
hvapt	36.50	kJ/mol	462.50	NIST Webbook
hvapt	35.40 ± 0.10	kJ/mol	396.00	NIST Webbook
hvapt	37.00 ± 0.10	kJ/mol	374.00	NIST Webbook
hvapt	35.36	kJ/mol	396.70	NIST Webbook
hvapt	38.80	kJ/mol	377.50	NIST Webbook
hvapt	38.40 ± 0.10	kJ/mol	354.00	NIST Webbook
hvapt	42.20	kJ/mol	349.00	NIST Webbook
hvapt	38.90	kJ/mol	380.50	NIST Webbook
hvapt	35.40	kJ/mol	547.00	NIST Webbook
rhol	813.00	kg/m3	295.00	KDB
sfust	4.70	J/mol×K	145.00	NIST Webbook
sfust	61.89	J/mol×K	217.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50365e+01
Coeff. B	-3.58989e+03
Coeff. C	-5.14190e+01
Temperature range (K), min.	294.82
Temperature range (K), max.	420.56

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.37823e+01
Coeff. B	-8.17241e+03
Coeff. C	-1.16608e+01
Coeff. D	7.67977e-06
Temperature range (K), min.	217.50
Temperature range (K), max.	582.82

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1202.mol
Measurements of activity coefficients at infinite dilution of organic solutes and water in 1-propyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide ionic liquid using GLC:	https://www.doi.org/10.1016/j.jct.2010.05.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The study of activity coefficients at infinite dilution for organic solutes and water in 1-butyl-4-methylpyridinium dicyanamide, [B4MPy][DCA] using GLC:	https://www.doi.org/10.1016/j.jct.2013.09.007
PPDS Method:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1202
Separation of aliphatic from aromatic hydrocarbons and sulphur compounds from fuel: Based on measurements of Activity Coefficients at Infinite Dilution of Solutes in Ionic Liquids Using Inverse Gas-Liquid Chromatography:	https://www.doi.org/10.1016/j.jct.2016.07.017
Determination of Activity Coefficients at Infinite Dilution for Organic Solutes and Water in the Ionic Liquid 1-Ethyl-1-methylpyrrolidinium Dicyanamide Using Inverse Gas-Liquid Chromatography:	https://www.doi.org/10.1021/acs.jced.8b00635
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589388&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Activity coefficients at infinite dilution for organic solutes and water in 1-ethyl-1-methylpyrrolidinium lactate:	https://www.doi.org/10.1016/j.jct.2015.05.014
Air-Water Partitioning of C5 and C6 Alkanones: Measurement, Critical Compilation, Correlation, and Recommended Data:	https://www.doi.org/10.1021/acs.jced.9b00726
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurements of activity coefficients at infinite dilution for organic solutes and water in 1-hexyl-1-methylpiperidinium dicyanamide using GLC:	https://www.doi.org/10.1016/j.jct.2013.02.004
Activity Coefficients at Infinite Dilution of Organic Solutes and Water in Tributylethylphosphonium Diethylphosphate Using Gas-Liquid Chromatography. Thermodynamic Properties of Mixtures Containing Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.5b00980
Activity coefficients at infinite dilution measurements for organic solutes and water in 1-ethyl-3-methylimidazolium ethylsulfate using GLC:	https://www.doi.org/10.1016/j.jct.2011.02.012
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Physicochemical properties and activity coefficients at infinite dilution for organic solutes and water in a novel bicyclic guanidinium superbase-derived protic ionic liquid:	https://www.doi.org/10.1016/j.jct.2012.09.033

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume