2-Hexanone, 5-methyl-

Other names:	(CH3)2CHCH2CH2COCH3
	2-Methyl-5-Hexanone
	3-Methylbutyl methyl ketone
	5-Methyl-2-hexanone
	5-Methylhexan-2-one
	ISOAMYL METHYL KETONE
	ISOPENTYL METHYL KETONE
	Ketone, methyl isoamyl
	MIAK
	Methyl isoamyl ketone
	Methyl isopentyl ketone
	UN 2302
Inchi:	InChI=1S/C7H14O/c1-6(2)4-5-7(3)8/h6H,4-5H2,1-3H3
InchiKey:	FFWSICBKRCICMR-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CC(=O)CCC(C)C
Mol. weight [g/mol]:	114.19
CAS:	110-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-123.30	kJ/mol	Joback Method
hf	-305.67	kJ/mol	Joback Method
hfus	11.96	kJ/mol	Joback Method
hvap	37.53	kJ/mol	Joback Method
ie	9.28 ± 0.01	eV	NIST Webbook
log10ws	-1.33		Aqueous Solubility Prediction Method
logp	2.012		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
pc	3022.28	kPa	Joback Method
rinpol	832.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	836.00		NIST Webbook

rinpol	830.90	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	831.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	828.00	NIST Webbook
rinpol	831.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	857.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	836.50	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	825.00	NIST Webbook
ripol	1172.10	NIST Webbook
ripol	1156.10	NIST Webbook
ripol	1160.90	NIST Webbook
ripol	1166.30	NIST Webbook
ripol	1150.00	NIST Webbook
ripol	1188.00	NIST Webbook
ripol	1168.00	NIST Webbook
ripol	1190.00	NIST Webbook
ripol	1155.00	NIST Webbook
ripol	1154.00	NIST Webbook
ripol	1186.00	NIST Webbook
ripol	1141.00	NIST Webbook
ripol	1146.00	NIST Webbook
ripol	1154.00	NIST Webbook
ripol	1140.00	NIST Webbook
ripol	1142.00	NIST Webbook

ripol	1156.00		NIST Webbook
tb	408.15 ± 2.00	K	NIST Webbook
tb	416.15 ± 2.00	K	NIST Webbook
tb	407.65 ± 2.00	K	NIST Webbook
tb	417.20	K	NIST Webbook
tb	418.05	K	NIST Webbook
tb	417.35 ± 1.00	K	NIST Webbook
tb	409.05 ± 1.00	K	NIST Webbook
tb	417.40 ± 0.50	K	NIST Webbook
tb	416.00 ± 5.00	K	NIST Webbook
tb	417.00 ± 3.00	K	NIST Webbook
tb	416.45 ± 1.00	K	NIST Webbook
tb	417.15 ± 2.00	K	NIST Webbook
tb	417.15 ± 2.00	K	NIST Webbook
tb	410.15 ± 2.00	K	NIST Webbook
tc	593.63	K	Joback Method
tf	199.25	K	NIST Webbook
tf	199.30 ± 0.60	K	NIST Webbook
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.47	J/mol×K	412.99	Joback Method
cpg	227.17	J/mol×K	443.10	Joback Method
cpg	238.41	J/mol×K	473.20	Joback Method
cpg	249.19	J/mol×K	503.31	Joback Method
cpg	259.52	J/mol×K	533.42	Joback Method
cpg	269.42	J/mol×K	563.52	Joback Method
cpg	278.88	J/mol×K	593.63	Joback Method
dvisc	0.0026700	Pa×s	238.48	Joback Method
dvisc	0.0065747	Pa×s	203.58	Joback Method
dvisc	0.0013648	Pa×s	273.38	Joback Method
dvisc	0.0008121	Pa×s	308.28	Joback Method
dvisc	0.0005371	Pa×s	343.19	Joback Method
dvisc	0.0003833	Pa×s	378.09	Joback Method
dvisc	0.0002897	Pa×s	412.99	Joback Method

rfi	1.40740		293.15	(Liquid + liquid) equilibria of (water + propionic acid + methyl isoamyl ketone or diisobutyl ketone or ethyl isoamyl keton) at T = 298.2 K
rfi	1.40510		293.20	Experimental and Correlational Study of Phase Equilibria in Aqueous Solutions of Formic and Butyric Acids with Isoamyl Acetate and Methyl Isoamyl Ketone at T = 298.15 K
rhol	887.90	kg/m3	293.20	Experimental study of phase equilibria in aqueous mixtures of phosphoric acid with isoamyl acetate and methyl isoamyl ketone at T = (298.2, 308.2, and 318.2) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53053e+01
Coeff. B	-3.82231e+03
Coeff. C	-5.73400e+01
Temperature range (K), min.	311.86
Temperature range (K), max.	439.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.08727e+02
Coeff. B	-9.25172e+03

Coeff. C	-1.38402e+01
Coeff. D	8.92111e-06
Temperature range (K), min.	199.25
Temperature range (K), max.	601.00

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
(Liquid + liquid) equilibria of (water + propionic acid + methyl isoamyl ketone or diisobutyl ketone or ethyl isoamyl keton) at T = 298.2 K:	https://www.doi.org/10.1016/j.fluid.2006.10.004
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110123&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Experimental and Correlational Study of Phase Equilibria in Aqueous Solutions of Formic and Butyric Acids with Isoamyl Acetate and Methyl Isoamyl Ketone at T = 298.15 K:	https://www.doi.org/10.1021/je401095k
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1209.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1209
Experimental study of phase equilibria in aqueous mixtures of phosphoric acid with isoamyl acetate and methyl isoamyl ketone at T = (298.2, 308.2, and 318.2) K:	https://www.doi.org/10.1016/j.fluid.2012.09.038

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
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
rfi:	Refractive Index
rhol:	Liquid 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