2-Octanone

Other names:	Hexyl methyl ketone
	Methyl hexyl ketone
	Methyl n-hexyl ketone
	N-HEXYL METHYL KETONE
	Octan-2-one
	Octanone-2
	n-C6H13COCH3
Inchi:	InChI=1S/C8H16O/c1-3-4-5-6-7-8(2)9/h3-7H2,1-2H3
InchiKey:	ZPVFWPFBNIEHGJ-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCCCCCC(C)=O
Mol. weight [g/mol]:	128.21
CAS:	111-13-7

Physical Properties

Property code	Value	Unit	Source
chl	-5070.20	kJ/mol	NIST Webbook
chl	-5050.13	kJ/mol	NIST Webbook
gf	-112.44	kJ/mol	Joback Method
hf	-345.10 ± 2.50	kJ/mol	NIST Webbook
hfus	18.07	kJ/mol	Joback Method
hvap	52.60	kJ/mol	NIST Webbook
hvap	39.80 ± 0.20	kJ/mol	NIST Webbook
hvap	51.80	kJ/mol	NIST Webbook
hvap	52.00 ± 0.30	kJ/mol	NIST Webbook
ie	9.75	eV	NIST Webbook
ie	9.40 ± 0.03	eV	NIST Webbook
ie	9.38	eV	NIST Webbook
log10ws	-2.05		Aqueous Solubility Prediction Method
log10ws	-2.05		Estimated Solubility Method
logp	2.546		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rhoc	257.71 ± 2.56	kg/m3	NIST Webbook
rinpol	999.00		NIST Webbook

rinpol	974.00	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	979.00	NIST Webbook
rinpol	974.00	NIST Webbook
rinpol	991.00	NIST Webbook
rinpol	969.00	NIST Webbook
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rinpol	968.00	NIST Webbook
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rinpol	990.00	NIST Webbook
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rinpol	1002.00	NIST Webbook
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ripol	1281.00		NIST Webbook
ripol	1269.00		NIST Webbook
ripol	1275.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1297.00		NIST Webbook
sl	373.84	J/mol×K	NIST Webbook
tb	436.31	K	Joback Method
tc	632.70 ± 0.20	K	NIST Webbook
tf	253.40	K	Vapour liquid equilibria, azeotropic data, excess enthalpies, activity coefficients at infinite dilution and solid liquid equilibria for binary alcohol ketone systems
tf	251.60 ± 0.40	K	NIST Webbook
tf	251.15 ± 0.50	K	NIST Webbook
tf	255.48	K	Aqueous Solubility Prediction Method
tt	252.79 ± 0.08	K	NIST Webbook
tt	252.86 ± 0.06	K	NIST Webbook
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.50	J/mol×K	436.31	Joback Method
cpg	267.99	J/mol×K	465.55	Joback Method
cpg	280.00	J/mol×K	494.78	Joback Method
cpg	291.52	J/mol×K	524.02	Joback Method
cpg	302.57	J/mol×K	553.25	Joback Method

cpg	313.17	J/mol×K	582.49	Joback Method
cpg	323.31	J/mol×K	611.72	Joback Method
cpl	273.26	J/mol×K	298.15	NIST Webbook
cpl	274.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0002948	Pa×s	436.31	Joback Method
dvisc	0.0020821	Pa×s	264.26	Joback Method
dvisc	0.0011762	Pa×s	298.67	Joback Method
dvisc	0.0007477	Pa×s	333.08	Joback Method
dvisc	0.0043730	Pa×s	229.85	Joback Method
dvisc	0.0003813	Pa×s	401.90	Joback Method
dvisc	0.0005173	Pa×s	367.49	Joback Method
hfust	24.42	kJ/mol	252.86	NIST Webbook
hfust	24.42	kJ/mol	252.90	NIST Webbook
hfust	24.42	kJ/mol	252.86	NIST Webbook
hvapt	49.80	kJ/mol	381.50	NIST Webbook
hvapt	49.10	kJ/mol	422.00	NIST Webbook
hvapt	50.60	kJ/mol	371.00	NIST Webbook
rhol	814.32	kg/m3	298.15	Excess molar enthalpies of binary systems containing 2-octanone, hexanoic acid, or octanoic acid at T = 298.15 K
rhol	819.90	kg/m3	293.15	Correlation of Experimental Liquid Liquid Equilibrium Data for Ternary Systems Using NRTL and GMDH-Type Neural Network
rhol	814.28	kg/m3	298.15	Excess Molar Enthalpies of Binary Systems of 2-Octanone or 3-Octanone with Dodecane, Tetradecane, or Hexadecane at 298.15 K
sfust	96.57	J/mol×K	252.86	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50683e+01
Coeff. B	-3.97956e+03
Coeff. C	-6.51800e+01
Temperature range (K), min.	334.42
Temperature range (K), max.	473.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.12914e+02
Coeff. B	-1.52457e+04
Coeff. C	-2.91025e+01
Coeff. D	1.72689e-05
Temperature range (K), min.	252.85
Temperature range (K), max.	624.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Excess molar enthalpies of binary systems containing 2-octanone, hexanoic acid, or octanoic acid at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.07.018
Correlation of Experimental Liquid-Liquid Equilibrium Data for Ternary Systems Using NRTL and UNIQUAC Type Local Models:	https://www.doi.org/10.1021/acs.jced.6b00985
Vapour-liquid equilibria, azeotropic data, excess enthalpies, activity coefficients at infinite dilution and solid-liquid equilibria for binary alcohol + ketone systems:	https://www.doi.org/10.1016/j.fluid.2008.02.021
Thermodynamic Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Liquid-Liquid Equilibria for Octan-2-one + Dihydroxybenzene + Water at Different Temperatures: Experimental Data and Thermodynamic Modeling:	https://www.doi.org/10.1021/acs.jced.9b00506
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1210
Excess Molar Enthalpies of Binary Systems of 2-Octanone or 3-Octanone with Dodecane, Tetradecane, or Hexadecane at 298.15 K:	https://www.doi.org/10.1021/je900311v
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Parametric Analysis of Mandelic Acid Separation from Aqueous Solutions by Using Secondary Amine Mixture (Amberlite LA-2) in Various Diluents:	https://www.doi.org/10.1021/acs.jced.9b00169
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1210.mol
A thermodynamic study of the ketoreductase-catalyzed reduction of 2-alkanones in non-aqueous solvents:	https://www.doi.org/10.1016/j.jct.2004.08.002
Thermodynamic Studies of Solubility for Naphthalene in 12 Solvents from 278 to 330 K:	https://www.doi.org/10.1021/acs.jced.9b00064
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111137&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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
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
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