2-Pentanone, 3-methyl-

Other names:	3-Methyl-2-pentanone
	3-Methylpentan-2-one
	Methyl 1-methylpropyl ketone
	Methyl sec-butyl ketone
	sec-Butyl Methyl ketone
	sec-C4H9COCH3
Inchi:	InChI=1S/C6H12O/c1-4-5(2)6(3)7/h5H,4H2,1-3H3
InchiKey:	UIHCLUNTQKBZGK-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCC(C)C(C)=O
Mol. weight [g/mol]:	100.16
CAS:	565-61-7

Physical Properties

Property code	Value	Unit	Source
gf	-131.72	kJ/mol	Joback Method
hf	-284.10 ± 1.30	kJ/mol	NIST Webbook
hfus	9.37	kJ/mol	Joback Method
hvap	41.50	kJ/mol	NIST Webbook
hvap	41.20	kJ/mol	NIST Webbook
hvap	40.59	kJ/mol	NIST Webbook
ie	9.69	eV	NIST Webbook
ie	9.21 ± 0.01	eV	NIST Webbook
ie	9.20 ± 0.05	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
ie	9.21 ± 0.01	eV	NIST Webbook
log10ws	-0.67		Estimated Solubility Method
log10ws	-0.67		Aqueous Solubility Prediction Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
rinpol	727.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	762.00		NIST Webbook

rinpol	751.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	735.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	735.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	735.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	736.84	NIST Webbook
rinpol	734.94	NIST Webbook
rinpol	732.26	NIST Webbook
rinpol	738.96	NIST Webbook
rinpol	734.80	NIST Webbook
rinpol	733.49	NIST Webbook
ripol	1033.90	NIST Webbook
ripol	1005.00	NIST Webbook
ripol	1067.00	NIST Webbook
ripol	1011.00	NIST Webbook
ripol	1016.00	NIST Webbook
ripol	1016.00	NIST Webbook
ripol	1019.00	NIST Webbook
ripol	1013.00	NIST Webbook
ripol	1014.00	NIST Webbook
ripol	1019.00	NIST Webbook
ripol	1016.00	NIST Webbook
ripol	1022.00	NIST Webbook
ripol	1034.00	NIST Webbook
ripol	1047.60	NIST Webbook
ripol	1020.00	NIST Webbook

ripol	1054.30		NIST Webbook
ripol	1040.80		NIST Webbook
ripol	1023.00		NIST Webbook
ripol	1013.00		NIST Webbook
tb	390.11	K	Joback Method
tc	571.90	K	NIST Webbook
tf	192.31	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.97 ± 0.28	J/mol×K	403.75	NIST Webbook
cpg	188.66 ± 0.28	J/mol×K	416.25	NIST Webbook
cpg	187.36 ± 0.28	J/mol×K	411.35	NIST Webbook
cpg	182.46 ± 0.27	J/mol×K	395.25	NIST Webbook
cpg	183.72 ± 0.28	J/mol×K	399.65	NIST Webbook
dvisc	0.0002910	Pa×s	390.11	Joback Method
dvisc	0.0005326	Pa×s	324.18	Joback Method
dvisc	0.0003828	Pa×s	357.14	Joback Method
dvisc	0.0061867	Pa×s	192.31	Joback Method
dvisc	0.0025603	Pa×s	225.28	Joback Method
dvisc	0.0013273	Pa×s	258.24	Joback Method
dvisc	0.0007984	Pa×s	291.21	Joback Method
hvapt	36.50	kJ/mol	420.00	NIST Webbook
hvapt	39.80	kJ/mol	343.00	NIST Webbook
hvapt	34.16	kJ/mol	390.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.20	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50153e+01
Coeff. B	-3.53784e+03
Coeff. C	-4.97230e+01
Temperature range (K), min.	289.94
Temperature range (K), max.	414.31

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.25886e+01
Coeff. B	-7.00758e+03
Coeff. C	-8.54893e+00
Coeff. D	6.48072e-06
Temperature range (K), min.	286.15
Temperature range (K), max.	415.15

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1200

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1200

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Air-Water Partitioning of C5 and C6 Alkanones: Measurement, Critical Compilation, Correlation, and Recommended Data: https://www.doi.org/10.1021/acs.jced.9b00726

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C565617&Units=SI

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

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume