3-Pentanone, 2-methyl-

Other names:	2-METHYL-3-PENTANONE
	2-Methyl-3-pentanal
	2-Methylpentan-3-one
	4-Methyl-3-pentanone
	Ethyl isopropyl ketone
	Isopropyl ethyl ketone
	iso-C3H7COC2H5
Inchi:	InChI=1S/C6H12O/c1-4-6(7)5(2)3/h5H,4H2,1-3H3
InchiKey:	HYTRYEXINDDXJK-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCC(=O)C(C)C
Mol. weight [g/mol]:	100.16
CAS:	565-69-5

Physical Properties

Property code	Value	Unit	Source
chl	-3750.16 ± 0.88	kJ/mol	NIST Webbook
gf	-131.72	kJ/mol	Joback Method
hf	-286.10 ± 0.90	kJ/mol	NIST Webbook
hfl	-325.90 ± 0.90	kJ/mol	NIST Webbook
hfus	9.37	kJ/mol	Joback Method
hvap	39.80 ± 0.20	kJ/mol	NIST Webbook
hvap	40.50	kJ/mol	NIST Webbook
hvap	39.79 ± 0.22	kJ/mol	NIST Webbook
ie	9.10 ± 0.01	eV	NIST Webbook
ie	9.10 ± 0.01	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
rinpol	734.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	733.00		NIST Webbook

rinpol	733.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	747.90		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	732.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	997.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	1003.00		NIST Webbook
ripol	972.00		NIST Webbook
ripol	989.00		NIST Webbook
ripol	1005.00		NIST Webbook
ripol	1003.00		NIST Webbook
ripol	1003.00		NIST Webbook
ripol	997.00		NIST Webbook
ripol	1003.00		NIST Webbook
tb	386.15 ± 2.00	K	NIST Webbook
tb	387.25 ± 1.00	K	NIST Webbook
tb	387.15 ± 1.00	K	NIST Webbook
tb	388.15 ± 1.00	K	NIST Webbook
tb	388.20 ± 1.00	K	NIST Webbook
tb	386.20	K	NIST Webbook
tb	387.70 ± 1.00	K	NIST Webbook
tb	386.15 ± 2.00	K	NIST Webbook
tb	386.00 ± 0.50	K	NIST Webbook
tb	387.65 ± 1.00	K	NIST Webbook
tb	388.15 ± 1.00	K	NIST Webbook
tb	389.00 ± 2.00	K	NIST Webbook
tb	387.90 ± 1.00	K	NIST Webbook
tb	387.15 ± 2.00	K	NIST Webbook
tb	390.15 ± 3.00	K	NIST Webbook
tb	390.65 ± 5.00	K	NIST Webbook
tb	368.15	K	NIST Webbook

tb	386.90 ± 1.00	K	NIST Webbook
tb	384.15 ± 3.00	K	NIST Webbook
tb	386.00 ± 3.00	K	NIST Webbook
tb	390.15 ± 1.00	K	NIST Webbook
tc	571.85	K	Joback Method
tf	192.31	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.77	J/mol×K	541.56	Joback Method
cpg	207.72	J/mol×K	480.98	Joback Method
cpg	198.11	J/mol×K	450.69	Joback Method
cpg	188.09	J/mol×K	420.40	Joback Method
cpg	177.67	J/mol×K	390.11	Joback Method
cpg	216.93	J/mol×K	511.27	Joback Method
cpg	234.22	J/mol×K	571.85	Joback Method
dvisc	0.0061867	Pa×s	192.31	Joback Method
dvisc	0.0002910	Pa×s	390.11	Joback Method
dvisc	0.0003828	Pa×s	357.14	Joback Method
dvisc	0.0005326	Pa×s	324.18	Joback Method
dvisc	0.0007984	Pa×s	291.21	Joback Method
dvisc	0.0013273	Pa×s	258.24	Joback Method
dvisc	0.0025603	Pa×s	225.28	Joback Method
hvapt	36.20	kJ/mol	413.50	NIST Webbook
hvapt	43.40	kJ/mol	343.50	NIST Webbook
hvapt	41.00	kJ/mol	333.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48028e+01
Coeff. B	-3.45648e+03
Coeff. C	-4.86110e+01
Temperature range (K), min.	286.74

Temperature range (K), max.	412.79

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.16937e+02
Coeff. B	-1.31300e+04
Coeff. C	-3.05877e+01
Coeff. D	2.58098e-05
Temperature range (K), min.	200.00
Temperature range (K), max.	567.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1203.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C565695&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1203
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Air-Water Partitioning of C5 and C6 Alkanones: Measurement, Critical Compilation, Correlation, and	https://www.doi.org/10.1021/acs.jced.9b00726
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Recommended Data:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume