3-Pentanone, 2,4-dimethyl-

Other names:	(iso-C3H7)2CO
	2,4-DIMETHYL-3-PENTANONE
	2,4-Dimethylpentan-3-one
	2,4-dimethyl-3-pentanone (diisopropyl ketone)
	Diisopropyl ketone
	ISOBUTYRONE
	Isopropyl ketone
	isobutyron
Inchi:	InChI=1S/C7H14O/c1-5(2)7(8)6(3)4/h5-6H,1-4H3
InchiKey:	HXVNBWAKAOHACI-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CC(C)C(=O)C(C)C
Mol. weight [g/mol]:	114.19
CAS:	565-80-0

Physical Properties

Property code	Value	Unit	Source
affp	850.30	kJ/mol	NIST Webbook
basg	820.50	kJ/mol	NIST Webbook
chl	-4402.50 ± 1.10	kJ/mol	NIST Webbook
gf	-125.74	kJ/mol	Joback Method
hf	-311.30 ± 1.10	kJ/mol	NIST Webbook
hfl	-352.90 ± 1.10	kJ/mol	NIST Webbook
hfus	8.44	kJ/mol	Joback Method
hvap	41.60 ± 0.10	kJ/mol	NIST Webbook
hvap	41.50 ± 0.08	kJ/mol	NIST Webbook
hvap	41.50 ± 0.10	kJ/mol	NIST Webbook
hvap	41.55 ± 0.07	kJ/mol	NIST Webbook
ie	8.95 ± 0.01	eV	NIST Webbook
ie	8.96 ± 0.01	eV	NIST Webbook
ie	8.96 ± 0.02	eV	NIST Webbook
ie	8.99 ± 0.04	eV	NIST Webbook
ie	8.94 ± 0.01	eV	NIST Webbook
log10ws	-1.30		Estimated Solubility Method
log10ws	-1.30		Aqueous Solubility Prediction Method

logp	1.868		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	778.00		NIST Webbook
rinpol	777.67		NIST Webbook
rinpol	779.36		NIST Webbook
rinpol	781.05		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	776.47		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	783.11		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	123.88		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	781.05		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	793.00		NIST Webbook
ripol	1041.00		NIST Webbook
ripol	1011.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1033.20		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	995.00		NIST Webbook
ripol	1033.20		NIST Webbook
ripol	1014.80		NIST Webbook
ripol	1020.80		NIST Webbook

ripol	1026.90		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	1011.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	1011.00		NIST Webbook
ripol	1007.00		NIST Webbook
sl	318.00	J/mol×K	NIST Webbook
tb	412.55	K	Joback Method
tc	597.41	K	Joback Method
tf	204.12 ± 0.05	K	NIST Webbook
tf	193.00 ± 6.00	K	NIST Webbook
tt	204.81 ± 0.07	K	NIST Webbook
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.96	J/mol×K	566.60	Joback Method
cpg	215.47	J/mol×K	412.55	Joback Method
cpg	227.54	J/mol×K	443.36	Joback Method
cpg	239.12	J/mol×K	474.17	Joback Method
cpg	250.20	J/mol×K	504.98	Joback Method
cpg	260.81	J/mol×K	535.79	Joback Method
cpg	280.65	J/mol×K	597.41	Joback Method
cpl	233.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0002786	Pa×s	412.55	Joback Method
dvisc	0.0114681	Pa×s	188.58	Joback Method
dvisc	0.0036989	Pa×s	225.91	Joback Method
dvisc	0.0016445	Pa×s	263.24	Joback Method
dvisc	0.0008942	Pa×s	300.56	Joback Method
dvisc	0.0005563	Pa×s	337.89	Joback Method
dvisc	0.0003803	Pa×s	375.22	Joback Method
hfust	11.20	kJ/mol	204.80	NIST Webbook
hfust	11.18	kJ/mol	204.81	NIST Webbook
hfust	11.20	kJ/mol	204.80	NIST Webbook
hvapt	39.40	kJ/mol	360.00	NIST Webbook

rfi	1.39740		298.15	Isothermal (vapour + liquid) equilibria in the binary and ternary systems composed of 2-propanol, 2,2,4-trimethylpentane, and 2,4-dimethyl-3-pentanone	
sfust	54.58	J/mol×K	204.81	NIST Webbook	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49262e+01
Coeff. B	-3.56992e+03
Coeff. C	-5.16690e+01
Temperature range (K), min.	295.54
Temperature range (K), max.	422.97

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isothermal (vapour + liquid) equilibria in the binary and ternary systems composed of 2-propanol, 2,2,4-trimethylpentane, and 2,4-dimethyl-3-pentanone:	https://www.doi.org/10.1016/j.jct.2011.09.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1207.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C565800&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
rfi:	Refractive Index
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