2-Pentanone, 4-hydroxy-4-methyl-

Other names:	(CH3)2C(OH)CH2C(O)CH3
	2-Hydroxy-2-methyl-4-pentanone
	2-Methyl-2-pentanol-4-one
	4-Hydroxy-2-keto-4-methylpentane
	4-Hydroxy-4-methyl-2-pentanone
	4-Hydroxy-4-methyl-pentan-2-on
	4-Hydroxy-4-methylpentan-2-one
	4-Hydroxy-4-methylpentanone-2
	4-Idrossi-4-metil-pentan-2-one
	4-Methyl-2-pentanon-4-ol
	4-Methyl-4-hydroxy-2-pentanone
	4-hydroxy-4-methyl-pentanone
	4-methyl-2-pentanone-4-ol
	Acetonyldimethylcarbinol
	Diacetonalcohol
	Diacetonalcool
	Diacetonalkohol
	Diacetone
	Diacetone alcohol
	Diacetone-alcool
	Diketone alcohol
	NSC 9005
	Pyranton
	Pyranton A
	Pyraton
	Tyranton
	UN 1148
Inchi:	InChI=1S/C6H12O2/c1-5(7)4-6(2,3)8/h8H,4H2,1-3H3
InchiKey:	SWXVUIWOUIDPGS-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC(=O)CC(C)(C)O
Mol. weight [g/mol]:	116.16
CAS:	123-42-2

Physical Properties

Property code	Value	Unit	Source

affp	822.90	kJ/mol	NIST Webbook
basg	791.10	kJ/mol	NIST Webbook
chl	-3483.30 ± 7.90	kJ/mol	NIST Webbook
gf	-263.26	kJ/mol	Joback Method
hf	-540.70	kJ/mol	NIST Webbook
hfl	-592.80 ± 7.70	kJ/mol	NIST Webbook
hfus	9.57	kJ/mol	Joback Method
hvap	52.13	kJ/mol	NIST Webbook
log10ws	-0.99		Crippen Method
logp	0.736		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	798.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	841.30		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	838.00		NIST Webbook

rinpol	848.00	NIST Webbook
rinpol	848.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	798.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1316.00	NIST Webbook
ripol	1369.00	NIST Webbook
ripol	1366.00	NIST Webbook
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ripol	1372.00	NIST Webbook
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ripol	1366.00	NIST Webbook
ripol	1369.00	NIST Webbook
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ripol	1366.00	NIST Webbook
ripol	1375.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1339.00	NIST Webbook
ripol	1339.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1390.00	NIST Webbook
ripol	1359.00	NIST Webbook
ripol	1376.00	NIST Webbook
ripol	1380.00	NIST Webbook

ripol	1358.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1343.00		NIST Webbook
tb	437.20	K	NIST Webbook
tb	439.20	K	NIST Webbook
tb	442.35	K	NIST Webbook
tb	442.35	K	NIST Webbook
tc	661.11	K	Joback Method
tf	230.35	K	NIST Webbook
tf	230.35	K	NIST Webbook
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.86	J/mol×K	479.50	Joback Method
cpg	270.68	J/mol×K	630.84	Joback Method
cpg	262.86	J/mol×K	600.57	Joback Method
cpg	254.59	J/mol×K	570.30	Joback Method
cpg	245.85	J/mol×K	540.04	Joback Method
cpg	236.61	J/mol×K	509.77	Joback Method
cpg	278.06	J/mol×K	661.11	Joback Method
dvisc	0.0081361	Pa×s	305.38	Joback Method
dvisc	0.0028958	Pa×s	340.20	Joback Method
dvisc	0.0012487	Pa×s	375.02	Joback Method
dvisc	0.0006212	Pa×s	409.85	Joback Method
dvisc	0.0003447	Pa×s	444.67	Joback Method
dvisc	0.0298236	Pa×s	270.55	Joback Method
dvisc	0.0002084	Pa×s	479.50	Joback Method
hvapt	51.00	kJ/mol	368.00	NIST Webbook
hvapt	47.50	kJ/mol	344.50	NIST Webbook

srf	0.03	N/m	323.15	Thermo Physical Properties of 4-Hydroxy 4-Methyl Pentanone with Nitrobenzene or Ethyl Benzene at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa
srf	0.03	N/m	323.15	Thermo Physical Properties of 4-Hydroxy 4-Methyl Pentanone with Nitrobenzene or Ethyl Benzene at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa
srf	0.03	N/m	313.15	Thermo Physical Properties of 4-Hydroxy 4-Methyl Pentanone with Nitrobenzene or Ethyl Benzene at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa
srf	0.03	N/m	303.15	Thermo Physical Properties of 4-Hydroxy 4-Methyl Pentanone with Nitrobenzene or Ethyl Benzene at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.78470e+01
Coeff. B	-5.91478e+03

Coeff. C	5.97000e+00
Temperature range (K), min.	330.88
Temperature range (K), max.	465.87

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123422&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility Measurement and Thermodynamic Modeling of Benzoic Acid in Monosolvents and Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.8b00025
Thermo-Physical Properties of 4-Hydroxy 4-Methyl Pentanone with Nitrobenzene at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa:	https://www.doi.org/10.1021/je8002699
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
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
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume