2-Pentanone, 4,4-dimethyl-

Other names:	4,4-Dimethyl-2-pentanone
	4,4-dimethylpentan-2-one
	Methyl neoamyl ketone
	Methyl neopentyl ketone
	Neopentyl methyl ketone
	neo-C5H11COCH3
Inchi:	InChI=1S/C7H14O/c1-6(8)5-7(2,3)4/h5H2,1-4H3
InchiKey:	AZASWMGVGQEVCS-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CC(=O)CC(C)(C)C
Mol. weight [g/mol]:	114.19
CAS:	590-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-118.02	kJ/mol	Joback Method
hf	-320.50 ± 1.90	kJ/mol	NIST Webbook
hfus	8.07	kJ/mol	Joback Method
hvap	36.63	kJ/mol	Joback Method
ie	9.23 ± 0.01	eV	NIST Webbook
log10ws	-1.79		Crippen Method
logp	2.012		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	750.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	750.00		NIST Webbook
ripol	1025.00		NIST Webbook
ripol	1025.00		NIST Webbook
tb	410.20	K	Joback Method
tc	598.48	K	Joback Method
tf	221.00	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.39	J/mol×K	410.20	Joback Method
cpg	230.12	J/mol×K	441.58	Joback Method
cpg	242.19	J/mol×K	472.96	Joback Method
cpg	253.64	J/mol×K	504.34	Joback Method
cpg	264.49	J/mol×K	535.72	Joback Method
cpg	274.76	J/mol×K	567.10	Joback Method
cpg	284.48	J/mol×K	598.48	Joback Method
dvisc	0.0067880	Pa×s	221.00	Joback Method
dvisc	0.0029812	Pa×s	252.53	Joback Method
dvisc	0.0015717	Pa×s	284.07	Joback Method
dvisc	0.0009417	Pa×s	315.60	Joback Method
dvisc	0.0006193	Pa×s	347.13	Joback Method
dvisc	0.0004367	Pa×s	378.67	Joback Method
dvisc	0.0003249	Pa×s	410.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49880e+01
Coeff. B	-3.58960e+03
Coeff. C	-5.18360e+01
Temperature range (K), min.	296.02
Temperature range (K), max.	422.80

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C590501&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

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
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