3-Pentanone, 2,2,4,4-tetramethyl-

Other names:	(t-C4H9)2CO
	2,2,4,4-Tetramethyl-3-pentanone
	2,2,4,4-Tetramethyl-pentan-3-one
	Di-tert-butyl ketone
	Hexamethylacetone
	Pivalone
Inchi:	InChI=1S/C9H18O/c1-8(2,3)7(10)9(4,5)6/h1-6H3
InchiKey:	UIQGEWJEWJMQSL-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CC(C)(C)C(=O)C(C)(C)C
Mol. weight [g/mol]:	142.24
CAS:	815-24-7

Physical Properties

Property code	Value	Unit	Source
affp	861.30	kJ/mol	NIST Webbook
basg	831.50	kJ/mol	NIST Webbook
chl	-5722.90 ± 1.10	kJ/mol	NIST Webbook
gf	-98.34	kJ/mol	Joback Method
hf	-345.80 ± 1.20	kJ/mol	NIST Webbook
hfl	-391.20 ± 1.20	kJ/mol	NIST Webbook
hfus	5.84	kJ/mol	Joback Method
hvap	45.40 ± 0.08	kJ/mol	NIST Webbook
hvap	45.40 ± 0.10	kJ/mol	NIST Webbook
hvap	45.35 ± 0.09	kJ/mol	NIST Webbook
hvap	45.50 ± 0.40	kJ/mol	NIST Webbook
hvap	45.40 ± 0.10	kJ/mol	NIST Webbook
ie	8.67 ± 0.02	eV	NIST Webbook
ie	8.67 ± 0.01	eV	NIST Webbook
ie	8.65 ± 0.03	eV	NIST Webbook
ie	8.71 ± 0.02	eV	NIST Webbook
ie	8.79 ± 0.05	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.648		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	900.00		NIST Webbook

rinpol	955.00		NIST Webbook
rinpol	916.70		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	916.70		NIST Webbook
rinpol	900.00		NIST Webbook
tb	452.73	K	Joback Method
tc	649.78	K	Joback Method
tf	247.91 ± 0.10	K	NIST Webbook
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.55	J/mol×K	452.73	Joback Method
cpg	318.74	J/mol×K	485.57	Joback Method
cpg	333.95	J/mol×K	518.41	Joback Method
cpg	348.22	J/mol×K	551.25	Joback Method
cpg	361.62	J/mol×K	584.10	Joback Method
cpg	374.18	J/mol×K	616.94	Joback Method
cpg	385.96	J/mol×K	649.78	Joback Method
dvisc	0.0097546	Pa×s	245.96	Joback Method
dvisc	0.0038032	Pa×s	280.42	Joback Method
dvisc	0.0018223	Pa×s	314.88	Joback Method
dvisc	0.0010096	Pa×s	349.35	Joback Method
dvisc	0.0006219	Pa×s	383.81	Joback Method
dvisc	0.0004149	Pa×s	418.27	Joback Method
dvisc	0.0002944	Pa×s	452.73	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50349e+01
Coeff. B	-3.80892e+03
Coeff. C	-5.93420e+01
Temperature range (K), min.	317.62
Temperature range (K), max.	451.07

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C815247&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
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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