3-Buten-2-one, 3-methyl-

Other names:	2-METHYL-1-BUTEN-3-ONE
	3- Methyl-3- butene-2- one
	3- Methyl-3- butene-2- one (methyl isopropenyl ketone)
	3-Methyl-3-buten-2-on
	3-Methyl-3-buten-2-one
	3-methylbut-3-en-2-one
	CH2=C(CH3)C(=O)CH3
	Isopropenyl methyl ketone
	Ketone, methyl isopropenyl
	Methyl isopropenyl ketone
	UN 1246
Inchi:	InChI=1S/C5H8O/c1-4(2)5(3)6/h1H2,2-3H3
InchiKey:	ZGHFDIIVVIFNPS-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C=C(C)C(C)=O
Mol. weight [g/mol]:	84.12
CAS:	814-78-8

Physical Properties

Property code	Value	Unit	Source
affp	843.10	kJ/mol	NIST Webbook
basg	811.30	kJ/mol	NIST Webbook
gf	-58.41	kJ/mol	Joback Method
hf	-143.47	kJ/mol	Joback Method
hfus	7.72	kJ/mol	Joback Method
hvap	32.88	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
nfpah	%!d(float64=2)		KDB
pc	3965.51	kPa	Joback Method
rinpol	643.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	653.00		NIST Webbook

rinpol	620.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	620.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	1006.00		NIST Webbook
ripol	991.00		NIST Webbook
ripol	987.00		NIST Webbook
ripol	1006.00		NIST Webbook
ripol	987.00		NIST Webbook
tb	371.20	K	NIST Webbook
tb	370.00 ± 3.00	K	NIST Webbook
tb	370.86 ± 0.20	K	NIST Webbook
tc	550.10	K	Joback Method
tf	219.55 ± 0.20	K	NIST Webbook
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.94	J/mol×K	364.23	Joback Method
cpg	137.08	J/mol×K	395.21	Joback Method
cpg	144.86	J/mol×K	426.19	Joback Method
cpg	152.29	J/mol×K	457.16	Joback Method
cpg	159.39	J/mol×K	488.14	Joback Method
cpg	166.17	J/mol×K	519.12	Joback Method
cpg	172.63	J/mol×K	550.10	Joback Method
hvapt	26.20	kJ/mol	342.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43966e+01
Coeff. B	-3.20200e+03
Coeff. C	-4.36900e+01
Temperature range (K), min.	270.64
Temperature range (K), max.	396.13

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.40040e+01
Coeff. B	-6.37294e+03
Coeff. C	-7.23558e+00
Coeff. D	4.27398e-06
Temperature range (K), min.	219.55
Temperature range (K), max.	566.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C814788&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1222
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1222.mol

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
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
nfpah:	NFPA Health Rating

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