Methyl vinyl ketone

Other names:	1-Buten-3-one
	2-Butenone
	3-Buten-2-one
	3-Butene-2-one
	3-Butenen-2-one
	3-Oxo-1-butene
	3-Oxobutene
	Acetone, methylene-
	Acetyl ethylene
	But-3-en-2-one
	Butenone
	CH2=CHCOCH3
	Ketone, methyl vinyl
	Methyl ethenyl ketone
	Methyl-vinyl-cetone
	Methylene acetone
	Methylvinylketon
	NSC 4853
	UN 1251
	Vinyl methyl ketone
	«gamma»-Oxo-«alpha»-butylene
	Â«gammaÂ»-Oxo-Â«alphaÂ»-butylene
Inchi:	InChI=1S/C4H6O/c1-3-4(2)5/h3H,1H2,2H3
InchiKey:	FUSUHKVFWTUUBE-UHFFFAOYSA-N
Formula:	C4H6O
SMILES:	C=CC(C)=O
Mol. weight [g/mol]:	70.09
CAS:	78-94-4

Physical Properties

Property code	Value	Unit	Source
affp	834.70	kJ/mol	NIST Webbook
basg	802.80	kJ/mol	NIST Webbook
gf	-58.28	kJ/mol	Joback Method
hf	-115.00 ± 11.00	kJ/mol	NIST Webbook
hfus	6.44	kJ/mol	Joback Method

hvap	30.57	kJ/mol	Joback Method
ie	9.61	eV	NIST Webbook
ie	10.11	eV	NIST Webbook
ie	9.66	eV	NIST Webbook
ie	9.67	eV	NIST Webbook
ie	9.66	eV	NIST Webbook
ie	9.65 ± 0.02	eV	NIST Webbook
ie	9.64	eV	NIST Webbook
log10ws	-0.63		Crippen Method
logp	0.761		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
rinpol	600.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	561.00		NIST Webbook
rinpol	561.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	581.00		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	568.20		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	576.00		NIST Webbook
ripol	946.00		NIST Webbook
ripol	931.00		NIST Webbook
ripol	942.00		NIST Webbook
ripol	995.00		NIST Webbook
ripol	946.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	948.00		NIST Webbook
ripol	947.00		NIST Webbook
ripol	953.00		NIST Webbook
ripol	947.00		NIST Webbook
ripol	947.00		NIST Webbook
ripol	961.00		NIST Webbook
ripol	927.00		NIST Webbook
ripol	932.00		NIST Webbook
ripol	943.00		NIST Webbook

ripol	938.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	932.00		NIST Webbook
ripol	947.00		NIST Webbook
ripol	953.00		NIST Webbook
sg	320.34	J/mol×K	NIST Webbook
tb	354.00 ± 4.00	K	NIST Webbook
tb	354.60	K	NIST Webbook
tc	523.88	K	Joback Method
tf	183.01	K	Joback Method
vc	0.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.50	J/mol×K	493.48	Joback Method
cpg	121.12	J/mol×K	463.08	Joback Method
cpg	115.48	J/mol×K	432.68	Joback Method
cpg	109.58	J/mol×K	402.27	Joback Method
cpg	103.42	J/mol×K	371.87	Joback Method
cpg	96.99	J/mol×K	341.47	Joback Method
cpg	131.64	J/mol×K	523.88	Joback Method
dvisc	0.0023375	Pa×s	183.01	Joback Method
dvisc	0.0002587	Pa×s	341.47	Joback Method
dvisc	0.0003201	Pa×s	315.06	Joback Method
dvisc	0.0004119	Pa×s	288.65	Joback Method
dvisc	0.0005576	Pa×s	262.24	Joback Method
dvisc	0.0008079	Pa×s	235.83	Joback Method
dvisc	0.0012851	Pa×s	209.42	Joback Method
hvapt	32.90	kJ/mol	317.00	NIST Webbook
hvapt	33.60	kJ/mol	327.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	309.80	K	19.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46500e+01
Coeff. B	-3.23247e+03
Coeff. C	-3.23750e+01
Temperature range (K), min.	257.44
Temperature range (K), max.	378.52

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78944&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume