2-Oxetanone, 4-methylene-

Other names:	3-Butenoic acid, 3-hydroxy-, «beta»-lactone
	3-Butenoic acid, 3-hydroxy-, Â«betaÂ»-lactone
	4-METHYLENE-2-OXETANONE
	DIKETENE
	DIMER
	Diketen
	ETHENONE
	Ethenone, dimer
	KETENE DIMER
	Vinylaceto-«beta»-lactone
	Vinylaceto-Â«betaÂ»-lactone
	but-3-en-3-olide
Inchi:	InChI=1S/C4H4O2/c1-3-2-4(5)6-3/h1-2H2
InchiKey:	WASQWSOJHCZDFK-UHFFFAOYSA-N
Formula:	C4H4O2
SMILES:	C=C1CC(=O)O1
Mol. weight [g/mol]:	84.07
CAS:	674-82-8

Physical Properties

Property code	Value	Unit	Source
chl	-1912.50 ± 0.42	kJ/mol	NIST Webbook
gf	-116.47	kJ/mol	Joback Method
hf	-190.20 ± 0.54	kJ/mol	NIST Webbook
hfl	-233.10 ± 0.46	kJ/mol	NIST Webbook
hfus	7.41	kJ/mol	Joback Method
hvap	42.90	kJ/mol	NIST Webbook
hvap	42.90	kJ/mol	NIST Webbook
hvap	42.90 ± 0.10	kJ/mol	NIST Webbook
hvap	42.90 ± 0.10	kJ/mol	NIST Webbook
ie	9.60 ± 0.02	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.447		Crippen Method
mcvol	59.500	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB

pc	5335.72	kPa	Joback Method
rinpol	709.20		NIST Webbook
tb	400.60	K	NIST Webbook
tb	399.20	K	NIST Webbook
tb	400.15	K	NIST Webbook
tc	616.42	K	Joback Method
tf	266.15 ± 2.00	K	NIST Webbook
vc	0.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.51	J/mol×K	400.53	Joback Method
cpg	113.46	J/mol×K	436.51	Joback Method
cpg	120.16	J/mol×K	472.49	Joback Method
cpg	126.61	J/mol×K	508.47	Joback Method
cpg	132.81	J/mol×K	544.46	Joback Method
cpg	138.75	J/mol×K	580.44	Joback Method
cpg	144.43	J/mol×K	616.42	Joback Method
hvapt	36.80	kJ/mol	399.20	NIST Webbook
hvapt	42.90	kJ/mol	342.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.70	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53129e+01
Coeff. B	-3.86501e+03
Coeff. C	-3.92000e+01

Temperature range (K), min.	266.65
Temperature range (K), max.	425.65

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.76192e+01
Coeff. B	-6.01856e+03
Coeff. C	-3.00236e+00
Coeff. D	3.40369e-07
Temperature range (K), min.	266.65
Temperature range (K), max.	616.00

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C674828&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=1218

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/research/kdb/hcprop/showprop.php?cmpid=1218

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

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

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume