Ketene

Other names:	CARBOMETHENE
	CH2CO
	ETHENONE
	Keto-ethylene
	METHYLENE KETONE
Inchi:	InChI=1S/C2H2O/c1-2-3/h1H2
InchiKey:	CCGKOQOJPYTBIH-UHFFFAOYSA-N
Formula:	C2H2O
SMILES:	C=C=O
Mol. weight [g/mol]:	42.04
CAS:	463-51-4

Physical Properties

Property code	Value	Unit	Source
af	0.2100		KDB
affp	822.90 ± 3.40	kJ/mol	NIST Webbook
affp	822.90 ± 3.40	kJ/mol	NIST Webbook
affp	825.30	kJ/mol	NIST Webbook
basg	790.10 ± 1.50	kJ/mol	NIST Webbook
basg	790.10 ± 1.50	kJ/mol	NIST Webbook
basg	793.60	kJ/mol	NIST Webbook
dm	1.40	debye	KDB
gf	-60.33	kJ/mol	KDB
hf	-61.84	kJ/mol	NIST Webbook
hf	-48.00 ± 2.00	kJ/mol	NIST Webbook
hf	-87.24	kJ/mol	NIST Webbook
hf	-61.13	kJ/mol	KDB
hfpi	879.00	kJ/mol	NIST Webbook
hfpiz	883.00	kJ/mol	NIST Webbook
hfus	6.99	kJ/mol	Joback Method
hvap	20.40 ± 5.90	kJ/mol	NIST Webbook
ie	9.61 ± 0.01	eV	NIST Webbook
ie	9.61 ± 0.02	eV	NIST Webbook
ie	9.61 ± 0.02	eV	NIST Webbook
ie	9.64	eV	NIST Webbook
ie	9.62 ± 0.00	eV	NIST Webbook
ie	9.62 ± 0.00	eV	NIST Webbook

ie	9.60	eV	NIST Webbook
ie	9.63 ± 0.02	eV	NIST Webbook
ie	9.64	eV	NIST Webbook
log10ws	-4.45		Crippen Method
logp	0.004		Crippen Method
mcvol	36.310	ml/mol	McGowan Method
pc	6500.00	kPa	KDB
tb	232.00	K	KDB
tc	380.00	K	KDB
tf	138.00	K	KDB
vc	0.145	m3/kmol	KDB
zc	0.2983050		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	46.15	J/mol×K	231.83	Joback Method
cpg	48.38	J/mol×K	256.49	Joback Method
cpg	50.52	J/mol×K	281.15	Joback Method
cpg	52.57	J/mol×K	305.81	Joback Method
cpg	54.53	J/mol×K	330.47	Joback Method
cpg	56.40	J/mol×K	355.13	Joback Method
cpg	58.19	J/mol×K	379.79	Joback Method
hvapt	20.63	kJ/mol	232.00	KDB
hvapt	20.40 ± 0.10	kJ/mol	191.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44321e+01
Coeff. B	-2.05785e+03
Coeff. C	-1.39620e+01
Temperature range (K), min.	159.45
Temperature range (K), max.	239.59

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1217.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C463514&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

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfpiz:	Enthalpy of formation of positive ion at 0K
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility