Acetyl chloride

Other names:	ACETIC CHLORIDE
	Acetic acid chloride
	Acetic acid monochloride
	CH3COCl
	ETHANOYL CHLORIDE
	Rcra waste number U006
	UN 1717
	UN1717 (DOT)
Inchi:	InChI=1S/C2H3ClO/c1-2(3)4/h1H3
InchiKey:	WETWJCDKMRHUPV-UHFFFAOYSA-N
Formula:	C2H3ClO
SMILES:	CC(=O)Cl
Mol. weight [g/mol]:	78.50
CAS:	75-36-5

Physical Properties

Property code	Value	Unit	Source
af	0.3440		KDB
aigt	663.15	K	KDB
dm	2.40	debye	KDB
fpo	277.59	K	KDB
gf	-206.40	kJ/mol	KDB
hf	-246.60	kJ/mol	NIST Webbook
hf	-251.30 ± 0.50	kJ/mol	NIST Webbook
hf	-244.00 ± 0.80	kJ/mol	NIST Webbook
hf	-244.10	kJ/mol	KDB
hfl	-272.00 ± 0.50	kJ/mol	NIST Webbook
hfl	-274.00 ± 0.59	kJ/mol	NIST Webbook
hfl	-275.20 ± 0.20	kJ/mol	NIST Webbook
hfus	6.73	kJ/mol	Joback Method
hvap	28.60	kJ/mol	NIST Webbook
hvap	23.80 ± 0.20	kJ/mol	NIST Webbook
ie	10.78	eV	NIST Webbook
ie	10.82 ± 0.04	eV	NIST Webbook
ie	11.02 ± 0.05	eV	NIST Webbook
ie	11.03	eV	NIST Webbook
ie	11.03	eV	NIST Webbook

ie	11.05	eV	NIST Webbook
ie	11.08 ± 0.06	eV	NIST Webbook
ie	10.85 ± 0.05	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	0.772		Crippen Method
mcvol	52.850	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=2)		KDB
pc	5870.00	kPa	KDB
rinpol	542.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	542.00		NIST Webbook
tb	324.00 ± 2.00	K	NIST Webbook
tb	324.10 ± 0.40	K	NIST Webbook
tb	324.20 ± 0.60	K	NIST Webbook
tb	324.40 ± 0.60	K	NIST Webbook
tb	325.20	K	NIST Webbook
tb	323.90	K	KDB
tb	324.00 ± 2.00	K	NIST Webbook
tb	324.00 ± 2.00	K	NIST Webbook
tb	324.00 ± 3.00	K	NIST Webbook
tb	328.00 ± 2.00	K	NIST Webbook
tb	325.00 ± 4.00	K	NIST Webbook
tc	508.00	K	KDB
tf	160.20	K	KDB
tf	161.20 ± 0.60	K	NIST Webbook
tf	160.29 ± 0.07	K	NIST Webbook
vc	0.204	m3/kmol	KDB
zc	0.2835100		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.90	J/mol×K	525.32	Joback Method
cpg	70.06	J/mol×K	336.46	Joback Method
cpg	80.61	J/mol×K	430.89	Joback Method
cpg	83.84	J/mol×K	462.36	Joback Method
cpg	86.94	J/mol×K	493.84	Joback Method
cpg	77.24	J/mol×K	399.41	Joback Method

cpg	73.72	J/mol×K	367.94	Joback Method
cpl	117.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0003359	Pa×s	336.46	Joback Method
dvisc	0.0005291	Pa×s	288.36	Joback Method
dvisc	0.0007065	Pa×s	264.31	Joback Method
dvisc	0.0009996	Pa×s	240.25	Joback Method
dvisc	0.0015279	Pa×s	216.20	Joback Method
dvisc	0.0004143	Pa×s	312.41	Joback Method
dvisc	0.0025970	Pa×s	192.15	Joback Method
hvapt	31.50	kJ/mol	295.50	NIST Webbook
hvapt	24.50	kJ/mol	298.00	NIST Webbook
hvapt	28.66	kJ/mol	323.90	KDB
hvapt	30.10 ± 0.42	kJ/mol	323.90	NIST Webbook
rhol	1104.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47561e+01
Coeff. B	-2.90110e+03
Coeff. C	-3.88330e+01
Temperature range (K), min.	239.34
Temperature range (K), max.	346.00

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C75365&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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1775.mol

Legend

af:	Acentric Factor
aigt:	Autoignition Temperature
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fpo:	Flash Point (Open Cup Method)
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility