Acetic acid, chloro-, ethyl ester

Other names:	2-Chloroacetic acid ethyl ester
	Acetic acid, 2-chloro-, ethyl ester
	Chloroacetic acid ethyl ester
	Ethyl chloracetate
	Ethyl chloroacetate
	Ethyl chloroethanoate
	Ethyl ester of chloroacetic acid
	Ethyl monochloracetate
	Ethyl monochloroacetate
	Ethyl «alpha»-chloroacetate
	Ethyl Â«alphaÂ»-chloroacetate
	Ethylester kyseliny chloroctove
	NSC 8833
	UN 1181
	chloroacetic acid, ethyl ester
	ethanoic acid, chloro-, ethyl ester
Inchi:	InChI=1S/C4H7ClO2/c1-2-7-4(6)3-5/h2-3H2,1H3
InchiKey:	VEUUMBGHMNQHGO-UHFFFAOYSA-N
Formula:	C4H7ClO2
SMILES:	CCOC(=O)CCl
Mol. weight [g/mol]:	122.55
CAS:	105-39-5

Physical Properties

Property code	Value	Unit	Source
chl	-2052.00	kJ/mol	NIST Webbook
gf	-263.05	kJ/mol	Joback Method
hf	-386.43	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	49.48	kJ/mol	NIST Webbook
hvap	49.47 ± 0.08	kJ/mol	NIST Webbook
hvap	49.50 ± 0.10	kJ/mol	NIST Webbook
log10ws	-0.51		Crippen Method
logp	0.788		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpol	776.00		NIST Webbook

rinpol	802.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	806.40		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	806.40		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	810.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1302.00		NIST Webbook
tb	404.64	K	Joback Method
tc	592.13	K	Joback Method
tf	236.92	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.84	J/mol×K	592.13	Joback Method
cpg	157.93	J/mol×K	435.89	Joback Method
cpg	151.10	J/mol×K	404.64	Joback Method
cpg	183.10	J/mol×K	560.88	Joback Method
cpg	177.14	J/mol×K	529.63	Joback Method
cpg	170.96	J/mol×K	498.39	Joback Method
cpg	164.55	J/mol×K	467.14	Joback Method

dvisc	0.0008979	Pa×s	308.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K
dvisc	0.0008341	Pa×s	313.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K
dvisc	0.0009692	Pa×s	303.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K
hvapt	45.00	kJ/mol	346.00	NIST Webbook
hvapt	40.43	kJ/mol	417.40	NIST Webbook
hvapt	48.50	kJ/mol	358.00	NIST Webbook
rfi	1.41730		303.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of Ethyl Chloroacetate + Cyclohexanone, + Chlorobenzene, + Bromobenzene, or + Benzyl Alcohol at (298.15, 303.15, and 308.15) K

rfi	1.42000		298.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of Ethyl Chloroacetate + Cyclohexanone, + Chlorobenzene, + Bromobenzene, or + Benzyl Alcohol at (298.15, 303.15, and 308.15) K
rfi	1.41480		308.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of Ethyl Chloroacetate + Cyclohexanone, + Chlorobenzene, + Bromobenzene, or + Benzyl Alcohol at (298.15, 303.15, and 308.15) K
rhol	1144.11	kg/m3	298.15	Excess molar volumes, viscosity deviations and excess thermal expansion coefficients for binary and ternary mixtures consist of diethylketone + 2-butanol + ethylchloroacetate at (298.15, 308.15 and 318.15) K

rhol	1131.46	kg/m3	308.15	Excess molar volumes, viscosity deviations and excess thermal expansion coefficients for binary and ternary mixtures consist of diethylketone + 2-butanol + ethylchloroacetate at (298.15, 308.15 and 318.15) K	
rhol	1118.74	kg/m3	318.15	Excess molar volumes, viscosity deviations and excess thermal expansion coefficients for binary and ternary mixtures consist of diethylketone + 2-butanol + ethylchloroacetate at (298.15, 308.15 and 318.15) K	
speedsl	1177.00	m/s	318.15	Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K	
speedsl	1198.00	m/s	313.15	Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K	

speedsl	1212.00	m/s	308.15	Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K
speedsl	1229.00	m/s	303.15	Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48407e+01
Coeff. B	-3.71707e+03
Coeff. C	-5.37270e+01
Temperature range (K), min.	309.14
Temperature range (K), max.	443.80

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
303.15	101.30	0.0012750

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Speeds of sound, isentropic compressibilities, viscosities, and excess molar volumes of binary mixtures of ethyl acetate with tetra- and trichloromethanes at 303.15 K:	https://www.doi.org/10.1016/j.tca.2004.07.014
Excess molar volumes, viscosity deviations and excess thermal pressure coefficients of binary and ternary mixtures consist of diethylketone + 2-butanol + ethylchloroacetate at (298.15, 308.15 and 318.15) K:	https://www.doi.org/10.1016/j.tca.2013.03.008
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Nist Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K:	https://www.doi.org/10.1021/je060343y
Volumetric and Transport Properties of Binary Liquid Mixtures of Methyl Methacrylate with Aliphatic Esters at Temperatures of (303.15 to 313.15) K:	https://www.doi.org/10.1021/je900525f
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of Ethyl Chloroacetate + Cyclohexanone, + Chlorobenzene, + Bromobenzene, or + Benzyl Alcohol at (298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je0201828
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume