Ethanol, 2-chloro-, acetate

Other names:	«beta»-Chloroethyl acetate
	1-Acetoxy-2-chloroethane
	2-Acetoxy-1-chloroethane
	2-Acetoxyethyl chloride
	2-Chloroethyl acetate
	CH3C(O)OCH2CH2Cl
	Acetic acid «beta»-chloroethyl ester
	2-Chloroethyl ethanoate
	Acetoxyethyl chloride
	2-Chlorethylacetat
	2-Chloroethanol acetate
	2-Chloroethyl ester of acetic acid
	Ethanol, 2-chloro-, 1-acetate
	NSC 77374
	Acetic acid, 2-chloroethyl ester
	Chloroethyl acetate
Inchi:	InChI=1S/C4H7ClO2/c1-4(6)7-3-2-5/h2-3H2,1H3
InchiKey:	VIRWKAJWTKAIMA-UHFFFAOYSA-N
Formula:	C4H7ClO2
SMILES:	CC(=O)OCCCl
Mol. weight [g/mol]:	122.55
CAS:	542-58-5

Physical Properties

Property code	Value	Unit	Source
gf	-263.05	kJ/mol	Joback Method
hf	-386.43	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	41.50 ± 0.20	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	825.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	816.00		NIST Webbook

rinpol	832.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	837.40		NIST Webbook
rinpol	837.40		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	796.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1341.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1341.00		NIST Webbook
tb	418.00	K	NIST Webbook
tb	418.20	K	NIST Webbook
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	151.10	J/mol×K	404.64	Joback Method
cpg	157.93	J/mol×K	435.89	Joback Method
cpg	164.55	J/mol×K	467.14	Joback Method
cpg	170.96	J/mol×K	498.39	Joback Method
cpg	177.14	J/mol×K	529.63	Joback Method
cpg	183.10	J/mol×K	560.88	Joback Method

cpg	188.84	J/mol×K	592.13	Joback Method
dvisc	0.0027868	Pa×s	236.92	Joback Method
dvisc	0.0016136	Pa×s	264.87	Joback Method
dvisc	0.0010371	Pa×s	292.83	Joback Method
dvisc	0.0007199	Pa×s	320.78	Joback Method
dvisc	0.0005298	Pa×s	348.73	Joback Method
dvisc	0.0004081	Pa×s	376.69	Joback Method
dvisc	0.0003259	Pa×s	404.64	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C542585&Units=SI
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

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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