

2-Propenoic acid, 2-chloroethyl ester

Other names:	Acrylic acid, 2-chloroethyl ester «beta»-Chloroethyl acrylate Acrylic acid «beta»-chloroethyl ester Chloroethyl acrylate 2-Chloroethyl acrylate Ethanol, 2-chloro-, acrylate 2-Chloroacrylic acid ethyl ester 2-Chlorethylester kyseliny akrylove 2-Chloroethyl ester of acrylic acid NSC 18592 NSC 65162
Inchi:	InChI=1S/C5H7ClO2/c1-2-5(7)8-4-3-6/h2H,1,3-4H2
InchiKey:	WHBAYNMEIXUTJV-UHFFFAOYSA-N
Formula:	C5H7ClO2
SMILES:	C=CC(=O)OCCCl
Mol. weight [g/mol]:	134.56
CAS:	2206-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-166.79	kJ/mol	Joback Method
hf	-281.64	kJ/mol	Joback Method
hfus	14.41	kJ/mol	Joback Method
hvap	39.59	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.954		Crippen Method
mcvol	96.690	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	424.20	K	Joback Method
tc	614.21	K	Joback Method
tf	246.43	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.64	J/molxK	424.20	Joback Method
cpg	179.18	J/molxK	455.87	Joback Method
cpg	186.44	J/molxK	487.54	Joback Method
cpg	193.40	J/molxK	519.21	Joback Method
cpg	200.06	J/molxK	550.88	Joback Method
cpg	206.45	J/molxK	582.54	Joback Method
cpg	212.54	J/molxK	614.21	Joback Method
dvisc	0.0026492	Paxs	246.43	Joback Method
dvisc	0.0015332	Paxs	276.06	Joback Method
dvisc	0.0009866	Paxs	305.69	Joback Method
dvisc	0.0006863	Paxs	335.32	Joback Method
dvisc	0.0005064	Paxs	364.94	Joback Method
dvisc	0.0003911	Paxs	394.57	Joback Method
dvisc	0.0003131	Paxs	424.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2206895&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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