2-Propenoic acid, 3-chloro-, (Z)-

Other names:	(Z)-3-Chloroacrylic acid
	cis-«beta»-Chloroacrylic acid
	cis-3-Chloroacrylic acid
	Acrylic acid, 3-chloro-, (Z)-
Inchi:	InChI=1S/C3H3ClO2/c4-2-1-3(5)6/h1-2H,(H,5,6)/b2-1-
InchiKey:	MHMUCYJKZUZMNJ-UPHRSURJSA-N
Formula:	C3H3ClO2
SMILES:	O=C(O)C=CCl
Mol. weight [g/mol]:	106.51
CAS:	1609-93-4

Physical Properties

Property code	Value	Unit	Source
gf	-223.07	kJ/mol	Joback Method
hf	-268.58	kJ/mol	Joback Method
hfus	13.61	kJ/mol	Joback Method
hvap	50.04	kJ/mol	Joback Method
log10ws	-0.68		Crippen Method
logp	0.823		Crippen Method
mcvol	68.510	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
tb	455.68	K	Joback Method
tc	646.19	K	Joback Method
tf	259.16	K	Joback Method
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.78	J/mol×K	455.68	Joback Method
cpg	117.08	J/mol×K	487.43	Joback Method
cpg	121.10	J/mol×K	519.18	Joback Method
cpg	124.87	J/mol×K	550.93	Joback Method
cpg	128.39	J/mol×K	582.68	Joback Method

cpg	131.68	J/mol×K	614.44	Joback Method
cpg	134.76	J/mol×K	646.19	Joback Method
dvisc	0.0224526	Pa×s	259.16	Joback Method
dvisc	0.0069569	Pa×s	291.91	Joback Method
dvisc	0.0027305	Pa×s	324.67	Joback Method
dvisc	0.0012720	Pa×s	357.42	Joback Method
dvisc	0.0006737	Pa×s	390.17	Joback Method
dvisc	0.0003937	Pa×s	422.93	Joback Method
dvisc	0.0002486	Pa×s	455.68	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1609934&Units=SI

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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