«alpha»-Chloroacrylic acid

Other names:	2-Chloroacrylic acid
	2-Propenoic acid, 2-chloro-
	Acrylic acid, 2-chloro-
	Alpha-chloroacrylic acid
Inchi:	InChI=1S/C3H3ClO2/c1-2(4)3(5)6/h1H2,(H,5,6)
InchiKey:	SZTBMYHIYNGYIA-UHFFFAOYSA-N
Formula:	C3H3ClO2
SMILES:	C=C(Cl)C(=O)O
Mol. weight [g/mol]:	106.51
CAS:	598-79-8

Physical Properties

Property code	Value	Unit	Source
gf	-224.00	kJ/mol	Joback Method
hf	-270.16	kJ/mol	Joback Method
hfus	10.82	kJ/mol	Joback Method
hvap	49.49	kJ/mol	Joback Method
log10ws	-0.68		Crippen Method
logp	0.823		Crippen Method
mcvol	68.510	ml/mol	McGowan Method
pc	5560.87	kPa	Joback Method
tb	448.08	K	Joback Method
tc	637.11	K	Joback Method
tf	248.52	K	Joback Method
vc	0.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.47	J/mol×K	448.08	Joback Method
cpg	118.68	J/mol×K	479.58	Joback Method
cpg	122.65	J/mol×K	511.09	Joback Method
cpg	126.39	J/mol×K	542.59	Joback Method
cpg	129.91	J/mol×K	574.10	Joback Method

cpg	133.23	J/mol×K	605.60	Joback Method
cpg	136.35	J/mol×K	637.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598798&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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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