2-Chloro-2-propen-1-ol

Other names:	«beta»-Chloroallyl alcohol
	2-Chloro-2-propenol
	2-Chloroallyl alcohol
	2-Propen-1-ol, 2-chloro-
	2-Chloro-3-hydroxypropene
Inchi:	InChI=1S/C3H5ClO/c1-3(4)2-5/h5H,1-2H2
InchiKey:	OSCXYTRISGREIM-UHFFFAOYSA-N
Formula:	C3H5ClO
SMILES:	C=C(Cl)CO
Mol. weight [g/mol]:	92.52
CAS:	5976-47-6

Physical Properties

Property code	Value	Unit	Source
gf	-95.08	kJ/mol	Joback Method
hf	-157.58	kJ/mol	Joback Method
hfus	9.22	kJ/mol	Joback Method
hvap	42.75	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.731		Crippen Method
mcvol	66.940	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
tb	406.70	K	NIST Webbook
tb	411.20	K	NIST Webbook
tc	571.26	K	Joback Method
tf	198.59	K	Joback Method
vc	0.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	108.02	J/mol×K	394.21	Joback Method
cpg	112.88	J/mol×K	423.72	Joback Method
cpg	117.51	J/mol×K	453.23	Joback Method

cpg	121.90	J/mol×K	482.74	Joback Method
cpg	126.08	J/mol×K	512.24	Joback Method
cpg	130.05	J/mol×K	541.75	Joback Method
cpg	133.82	J/mol×K	571.26	Joback Method

Sources

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=C5976476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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